TRANSPORT EQUATIONS FOR ELECTRONS AND PHONONS

K. H. MICHEL

TRANSPORT EQUATIONS FOR ELECTRONS AND PHONONS

Promotor: PROF. DR. IR. E. VERBOVEN

TRANSPORT EQUATIONS FOR ELECTRONS AND PHONONS

PROEFSCHRIFT

TER VERKRIJGING VAN DE GRAAD VAN DOCTOR
IN DE WISKUNDE EN NATUURWETENSCHAPPEN
AAN DE KATHOLIEKE UNIVERSITEIT TE NIJMEGEN,
OP GEZAG VAN DE RECTOR MAGNIFICUS DR. W. J. M. A. ASSELBERGS,
HOOGLERAAR IN DE FACULTEIT DER LETTEREN,
VOLGENS HET BESLUIT VAN DE SENAAT
IN HET OPENBAAR TE VERDEDIGEN OP VRIJDAG 22 JANUARI 1965,
DES NAMIDDAGS TE 2 UUR

DOOR

KARL-HEINZ MICHEL

GEBOREN 7 JUNI 1939 TE EUPEN (BELGIË)

KONINKLIJKE DRUKKERIJ VAN DE GARDE N.V.
ZALTBOMMEL

Meiner Mutter

CONTENTS

CHAPTER 1

INTRODUCTION AND SUMMARY

The description of transport phenomena for electrons and phonons in metals and semiconductors has usually been based on a Boltzmann equation approach. In doing so one assumes that the electron and the phonon distribution functions $f^e(\boldsymbol{k})$ and $f^p(\boldsymbol{q})$ satisfy the equations

$$\frac{\partial f^e}{\partial t}(\boldsymbol{k}, t) = -\frac{eE}{m}\frac{\partial f^e}{\partial \boldsymbol{k}}(\boldsymbol{k}, t) + \left(\frac{\partial f^e}{\partial t}\ \boldsymbol{k}, t\right)_{\text{coll.}} \tag{1}$$

$$\frac{\partial f^p}{\partial t}(\boldsymbol{q}, t) = \left(\frac{\partial f^p}{\partial t}(\boldsymbol{q}, t)\right)_{\text{coll}} \tag{2}$$

The first term on the right-hand side of (1) gives the change of the electron distribution due to the external electric field $\boldsymbol{E}$ (e being the electron charge, m its mass and $\boldsymbol{k}$ its momentum), the second term describes the change of f^e due to the collision of the electrons with the phonons of the lattice.

Equation (2) for the phonon distribution $f^p(\boldsymbol{q})$, ($\boldsymbol{q}$ being the phonon wave vector) assumes that there is no direct effect of the external field and the phonons are only driven out from equilibrium via their collisions with the electrons. In the steady state case, the left-hand side term of (1) vanishes and the r.h.s. terms show that the effect of the external field is counterbalanced by the electron phonon collisions. By solving equation (1) and retaining only terms linear in the electric field, one takes for $f^e(\boldsymbol{k})$ in the first r.h.s. term of (1) the unperturbed Fermi-Dirac distribution $f_0^e(\boldsymbol{k})$ while the collision term is calculated usually by second order perturbation theory. The collision term in eq. (2) for phonons is evaluated in the same manner. As a result one obtains the well known Boltzmann equations for electrons and phonons[1]), which are of second order in the electron-phonon coupling λ_q. The approach just described may be subject to several critics[1])[2]).

A first weakness is the treatment of the collision terms in eq. (1) and (2). The transition probabilities needed therefore are derived by means of lowest order time dependent perturbation theory which is only correct for sufficiently short time intervals Δt. The use of the time independent tran-

sition probabilities at any time t in the collision term is then made plausible by arguments involving randomization of phases and assumptions about the duration of the collisions. In particular, one assumes that the duration of a collision is shorter than the time between successive collisions. In connexion with the latter approximation, we are led to consider another difficulty of the usual Boltzmann equation. By writing down eq. (1), one assumes that the collision term is not influenced by the external field, in other words, the external field is considered to act only on particles which propagate freely in between collisions, and one neglects the action of the field *during* the collisions.

In order to avoid the previously mentioned difficulties and to give a more correct treatment of transport phenomena, one has to start from other basic expressions than eq. (1) and (2).

A general formula describing the response of a system to an external perturbation, has been given by Kubo[3]). His treatment is based on the consideration of the change due to the external field, of the density matrix of the system.

If the external perturbation is sufficiently weak, one is allowed to consider only the linear response function which can be expressed in terms of a two time correlation function. In particular, the electrical conductivity is written as a two currents correlation function. This type of Kubo formula was used by Chester and Thellung[4]) and also by Verboven[5]) in considering transport phenomena for the case of electron-impurity scattering. The same problem was studied by Kohn and Luttinger[6]) by a different approach, based on the one electron density matrix. In all these investigations, the situation was considerably simplified by the fact that one was allowed to consider only one electron interacting with a system of randomly distributed static impurities.

In the case of electron-phonon scattering, the situation is more complicated. One deals with a real many body problem and the techniques used in the previous papers are less convenient.

In the last years, field theoretical methods have been applied with great success in solid state physics and in statistical mechanics. The Green's function (or propagator) techniques revealed to be the most powerful and effective method, applicable to both equilibrium and transport problems in statistical physics[7]).

In chapter II of the present study, we don't consider the Kubo formula in its usual form, but we start from an expression which appears already in an early stage of the derivation of Kubo's formula. This permits to write directly the electrical conductivity in terms of the Fourier transform of a retarded Green's function G_k. This Green's function can be interpreted as the change, due to the applied external field, of the electron distribution; it plays the role of the deviation (linear in $\boldsymbol{E}$) of the function f^e_k in the usual

Boltzmann equation (1) with respect to its equilibrium value $f_0^e(\boldsymbol{k})$. Starting from such a "simple" Geen's function $G_{\boldsymbol{k}}$, and applying then the equation of motion method for Green's function, we construct the hierarchy of G.F. involving mixed electron-phonon G.F. of increasing order. As is known from the general theory, one has to truncate the hierarchy by some approximation method. In our problem we close at once the hierarchy by the so called decoupling techniques, a method first applied by Bogoljubov and Tyablikov[7][8] and inspired from classical statistical mechanics. In this way, we obtain a linear integral equation for $G_{\boldsymbol{k}}$ involving also $D_{\boldsymbol{q}}$, the deviation from equilibrium of the phonon distribution. The latter effect, which comes out naturally in our calculations, is usually known as phonon drag. The Green's function $D_{\boldsymbol{q}}$ satisfies in turn an integral equation which contains also $G_{\boldsymbol{k}}$. In the case of a static electric field, our system of two coupled integral equations is equivalent to a linearized version of the Bloch-Boltzmann equations for both electrons and phonons including phonon drag terms[1]. The inhomogeneous term in the equation for $G_{\boldsymbol{k}}$ is identical with the usual streaming term of the Boltzmann equation while the homogeneous part corresponds to the collision term and is of second order in the electron-phonon coupling $\lambda_{\boldsymbol{q}}$. This shows claerly that the separation between streaming and collision, as made in eq. (1), is justified in lowest order of the electron-phonon interaction. The last sections of chapter II are devoted to the discussion of conservation laws for energy, total momentum and number of electrons. The conservation laws are given as well for the exact kinetic equations (to any order in the electron-phonon coupling) as well as for the kinetic equations obtained after decoupling. In the absence of "Umklapprozesse", the total momentum is a conserved quantity and the electrical conductivity becomes infinite. This is a well known consequence of the phonon drag[1]. Finally, kinetic equations are given by including "Umklapprozesse". It is then shown how the conservation laws are modified and therefore the electrical conductivity remains finite.

The following chapter is an extension to higher order in the electron-phonon coupling. At first the hierarchy of Green's functions is developed to fourth order. Decoupling at this stage yields again the results of order λ_q^2 given in chapter II and additional terms which are of higher order (λ_q^4) in the electron-phonon interaction. Two main classes of corrections are obtained.

First there are the collision term corrections (order λ_q^4) which are given by the homogeneous part of the integral equation. Here again one may distinguish between two groups. A first part of terms, which are build up form products of lowest order matrix elements, takes into account the renormalization of the electron and phonon energies and corrections to the transition probabilities. The remaining part of collision term corrections contains mixed electron-phonon density matrices, taking into account correlation effects specific to the many body character of the system.

The second class of corrections is of entirely different nature and merits special interest. Indeed, in the equation for the electron Green's function G_k one obtains in addition to the usual streaming term, mentioned in the previous chapter, a whole class of terms which may be seen as arising from interference between steaming and collision. These terms belong to the inhomogeneous part of the integral equation and are proportional to the external perturbation, they would not exist in absence of the external perturbation (for instance in a system which relaxes to equilibrium). On the other hand, they are also proportional to the electron-phonon interaction (in our case of order λ_q^2), and contain other factors arising from collision. These interference terms are due to the action of the electric field during collisions. Here the particles are no longer seen as propagating freely in between instantaneous collisions. Contributions of the same nature appear also in the kinetic equation for phonons which is generally (in lowest order considered without streaming term. Our results show that the sheme given by eq. (1) and (2) is justified only in lowest order in the particle interaction and that it breaks down in a more correct formulation of transport phenomena.

Chapters II and III are published as separate articles in Physica, Physica **30**, 410 (1964) and 2194 (1964).

Acknowledgements. The author is greatly indebted to Dr. J. M. J. Van Leeuwen for the very pleasant collaboration in the first part of this work and for useful suggestions and comments.

REFERENCES

1) Peierls, R. E., Quantum Theory of Solids, Oxford (1955) pag. 127.
2) Fröhlich, H. and Taylor, A. W. B., Proc. Phys. Soc., **83** (1964) 739.
3) Kubo, R., J. Phys. Soc. Japan **12** (1957) 570.
4) Chester, G. V. and Thellung, A., Proc. Phys. Soc. **73** (1959) 745.
5) Verboven, E., Physica **26** (1960) 1091.
6) Kohn, W. and Luttinger, J. M., Phys. Rev. **108** (1957) 590.
7) Zubarev, D. N., Sov. Phys. Uspekhi **3** (1960) 320.
Bonch-Bruevich, V. L. and Tyablikov, S. V., The G.F. method in statistical mechanics, Northholland (1962).
8) Bogoljubov, N. N. and Tyablikov, S. V., Sov. Phys. Doklady **4** (1959) 589.

CHAPTER II

GREEN'S FUNCTION APPROACH TO ELECTRICAL CONDUCTIVITY AND PHONON DRAG

Synopsis

The Kubo expression for the frequency dependent electrical conductivity $\sigma(\omega)$ of a system of electrons interacting with phonons by the Frohlich Hamiltonian, is studied by many body Green's function theory. The contributions of lowest order in the electron-phonon coupling to $\sigma(\omega)$ are obtained by deriving equations of motion for Green's functions and applying decoupling techniques They have to be calculated from the solution of a set of two coupled kinetic equations for both the electron and the phonon distribution functions in which the so called phonon drag appears in a natural way. In the particular case of a static electrical field ($\omega = 0$), the set of equations reduces to two linearized Boltzmann equations. As a consequence of the phonon drag terms (being of lowest order in the coupling), this set has no finite solution, "Umklapprozesse" being neglected. The static electrical conductivity tensor then becomes infinite. Furthermore it is stressed that the phonon drag occurs also in the case of the low electron density limit If one considers Umklapprozesse, supplementary terms appear in the kinetic equations, which prevent the electric conductivity to become infinite for zero frequency.

1. *Introduction.* The calculation of the electrical conductivity of electrons in crystalline solids has obtained a renewed attention since the work of Kubo[1]), who derived expressions of great generality for the linear response of a system to an external perturbation. Although the Kubo expression for the conductivity is well defined, its calculation is by no means straightforward. In the case where the resistance is due to the scattering of the electrons by static impurities, the Kubo expression can be reduced to a one electron formula. Starting from this point of view, Verboven[2]) could give a development of the electrical conductivity tensor in powers of the electron-impurity coupling. On the other hand, if one considers the case where the electrons are scattered by the lattice waves (phonons), the situation becomes more complicated. Here the motion of one electron cannot be separated from the others because of their mutual interaction through the phonon field, and thus one has to deal with a real many body problem.

The electrical conductivity of a system of electrons and phonons described

by the Fröhlich Hamiltonian has recently been investigated by Fujita and Abe[3]). Using a diagram representation for the real time Green's functions, these authors calculate in a systematic way the lowest order contribution to the static electrical consductivity tensor. The conductivity follows from the solution of an integral equation of the same type as one would obtain from a linearized Boltzmann theory.

To our opinion, however, this treatment is incomplete because the induced deviation of the phonon distribution (phonon drag), which is also a lowest order effect, is not taken into account. In this chapter we show the importance of this effect for a systematic calculation of the electrical conductivity in powers of the electron-phonon coupling. It turns out that we have to calculate the conductivity from a coupled set of linear kinetic equations for the deviation from equilibrium of both the electron and the phonon distribution functions. The calculations are made for an external electric field of frequency ω. For the case $\omega = 0$, the results are in agreement with the linearized Boltzmann equations derived in the conventional way and also derived by Lang[4]) using techniques developed by Kohn and Luttinger[5]).

We start (section 2) from a Kubo formula which leads immediately to the concept of a retarded Green's function, determining the deviation from equilibrium of the one electron distribution function. In section 3 this Green's functions is studied by deriving the equations of motion for the Green's functions, in which lower order Green's functions are expressed in terms of higher order Green's functions. These higher order Green's functions are decoupled by expressing them in terms of lower order ones (section 4) and so we get a system of two coupled linear kinetic equations. In section 5 the conservation of electron number, total momentum and energy are considered. It is stressed that the conductivity becomes infinite for zero frequency if one does not take into account the so called Umklapprozesse. Finally the kinetic equations are derived by including Umklapprozesse (section 6).

2. *Formulation of the problem.* Since the fundamental paper of Kubo[1]), it is known that quantities which characterize the linear response of a system to an external perturbation, are given by expressions containing only averages over the unperturbed ensemble. In particular for the electrical conductivity which appears as the linear response coefficient with respect to an electric field, there exist many equivalent expressions, obtained after more or less complicated manipulations. For our purpose it is most convenient to start from an expression which appears already in an early stage of the derivation of Kubo's formula[6])[7]). We shall briefly recall some details on this point.

Let the ensemble, characterized by the Hamiltonian $\mathscr{H}$, be initially in

equilibrium. At a time $t = -\infty$, an external perturbation $\Delta\mathscr{H}$ is switched on, given by the expression

$$\Delta\mathscr{H} = -A \exp(-i\omega t + \varepsilon t)\mathscr{C}_1. \tag{2.1}$$

Here A is the amplitude of the external field of frequency ω and $\mathscr{C}_1$ describes the coupling between the ensemble and the external perturbation. The deviation $\Delta\langle\mathscr{C}_2\rangle_{t'}$, of the average value of an operator $\mathscr{C}_2$ at time t', due to the perturbation, is then to first order in A given by

$$\Delta\langle\mathscr{C}_2\rangle_{t'} = iA\int_{-\infty}^{+\infty} \mathrm{d}t\, \theta(t'-t)\, \langle[\mathscr{C}_2(t'), \mathscr{C}_1(t)]\rangle \exp(-i\omega t + \varepsilon t). \tag{2.2}$$

$\theta(t'-t)$ is the usual step function being 0 for $t' < t$ and 1 for $t' > t$, the bracket $\langle\ \rangle$ denotes an average value with respect to the equilibrium ensemble i.e. without external perturbation. The operators $\mathscr{C}_2(t')$ and $\mathscr{C}_1(t)$ are written in Heisenberg representation with respect to the Hamiltonian $\mathscr{H}$. Let us consider expression (2.2) at time $t' = 0$. From (2.2) it is then easy to obtain the following formula

$$\Delta\langle\mathscr{C}_2\rangle_{t'=0} = iA\int_{-\infty}^{+\infty} \mathrm{d}t\, \theta(t)\, \langle[\mathscr{C}_2(t), \mathscr{C}_1(0)]\rangle \exp(i\omega t - \varepsilon t). \tag{2.3}$$

At this point it is convenient to introduce the notion of a retarded Green's function for two operators $\mathscr{C}_2$ and $\mathscr{C}_1$ (for more details see ref. 6):

$$\ll\mathscr{C}_2; \mathscr{C}_1\gg_t = -i\theta(t)\, \langle[\mathscr{C}_2(t), \mathscr{C}_1(0)]\rangle. \tag{2.4}$$

If we define the Fourier transform of (2.4) by

$$\ll\mathscr{C}_2; \mathscr{C}_1\gg_\omega = \frac{1}{2\pi}\int_{-\infty}^{+\infty} \mathrm{d}t\, \ll\mathscr{C}_2; \mathscr{C}_1\gg_t \exp(i\omega t), \tag{2.5}$$

equation (2.3) becomes

$$\Delta\langle\mathscr{C}_2\rangle_{t'=0} = -2\pi A\, \ll\mathscr{C}_2; \mathscr{C}_1\gg_{\omega+i\varepsilon}. \tag{2.6}$$

The expression

$$\chi_{\mathscr{C}_1, \mathscr{C}_2}(\omega) = -2\pi\, \ll\mathscr{C}_2; \mathscr{C}_1\gg_{\omega+i\varepsilon} \tag{2.7}$$

is usually called the complex admittance. Formulas (2.1), (2.7) are quite general and not restricted to a specific system.

For our particular problem of electrons in a crystal, the system is described by the Fröhlich Hamiltonian

$$\mathscr{H} = \sum_k E_k\, a_k^\dagger a_k + \sum_q \omega_q b_q^\dagger b_q + \sum_{k,q} \lambda_q\, a_{k+q}^\dagger a_k (b_q + b_{-q}^\dagger). \tag{2.8}$$

Here $a_k^\dagger$, a_k, are the creation and annihilation operators for an electron in the state $|k\rangle$, E_k is the kinetic energy of a free electron while $b_q^\dagger$, b_q and ω_q are the corresponding quantities for phonons ($\hbar = 1$). The summation over

q runs over the first Brillouin zone, while the k- sum runs over the whole momentum space. The function λ_q with the property $\lambda_q = \lambda_{-q}$ determines the coupling between electrons and phonons. In the case of electrical conductivity, the external perturbation is given by an electric field $\boldsymbol{E} \exp(-i\omega t + \varepsilon t)$ of frequency ω. The perturbation Hamiltonian $\Delta\mathscr{H}$ has the form

$$\Delta\mathscr{H} = -\boldsymbol{E}\cdot e\,\mathscr{D} \exp(-i\omega t + \varepsilon t) \tag{2.9}$$

where $e\mathscr{D}$ is the total dipole moment of the system, e being the one electron charge, while the ν-th component of $\mathscr{D}$ is given by

$$\mathscr{D}_\nu = \int r_\nu\, \psi^\dagger(r)\, \psi(r)\, \mathrm{d}r. \tag{2.10}$$

The operators $\psi^\dagger(r)$ are related to the $a_k^{(\dagger)}$ by

$$\psi(r) = \sum_k a_k \langle r|k\rangle,\quad \psi^\dagger(r) = \sum_k a_k^\dagger \langle k|r\rangle, \tag{2.11}$$

where $\langle r|k\rangle$ is the wave function of the state $|k\rangle$. We see that $e\mathscr{D}$ plays the role of the operator $\mathscr{C}_1$ while the operator $\mathscr{C}_2$ is here the current $\mathscr{J}$. The latter is an additive operator and we write its μ-th component in the form

$$\mathscr{J}_\mu = \sum_k (j_k)_\mu\, a_k^\dagger a_k. \tag{2.12}$$

Here $(j_k)_\mu$ is the μ-th component of the one electron current operator which is diagonal in the k-representation. The admittance now corresponds to the electric conductivity tensor $\sigma_{\mu\nu}(\omega)$ given by

$$\sigma_{\mu\nu}(\omega) = -\frac{2\pi e}{V} \langle\langle \mathscr{J}_\mu;\, \mathscr{D}_\nu \rangle\rangle_{\omega+i\varepsilon} \tag{2.13}$$

(V is the volume of the system).

By inserting (2.12) into (2.13) one obtains

$$\sigma_{\mu\nu}(\omega) = -\frac{2\pi e}{V} \sum_k (j_k)_\mu \langle\langle a_k^\dagger a_k;\, \mathscr{D}_\nu \rangle\rangle_{\omega+i\varepsilon}. \tag{2.14}$$

The interpretation of the function $\langle\langle a_k^\dagger a_k;\, \mathscr{D}_\nu \rangle\rangle_{\omega+i\varepsilon}$ follows from (2.6) when we take for $\mathscr{C}_2$ the operator $a_k^\dagger a_k$ giving the distribution of the electrons in the state $|k\rangle$. So we have for the deviation $\Delta\langle a_k^\dagger a_k\rangle_{t'=0}$ of the average electron distribution according to (2.6)

$$\Delta\langle a_k^\dagger a_k\rangle_{t'=0} = -2\pi e\, \boldsymbol{E}\cdot \langle\langle a_k^\dagger a_k;\, \mathscr{D}_\nu \rangle\rangle_{\omega+i\varepsilon} \tag{2.15}$$

Thus from the Boltzmann theory approach it may be expected that $\langle\langle a_k^\dagger a_k;\, \mathscr{D}_\nu \rangle\rangle_{\omega+i\varepsilon}$ has to be found from a Boltzmann equation linearized in the external field.

3. *The equations of motion.* By differentiating the Green's function defined by (2.4) with respect to t we get the following equation of motion:

$$i\frac{\mathrm{d}}{\mathrm{d}t}\langle\langle \mathscr{C}_2; \mathscr{C}_1\rangle\rangle_t = \delta(t)\,\langle[\mathscr{C}_2(t), \mathscr{C}_1(t)]\rangle + \langle\langle[\mathscr{C}_2, \mathscr{H}]; \mathscr{C}_1\rangle\rangle_t. \tag{3.1}$$

Here $\mathscr{H}$ is the Hamiltonian without the external perturbation $\Delta\mathscr{H}$. In terms of Fourier transforms, (3.1) becomes

$$\omega\langle\langle \mathscr{C}_2; \mathscr{C}_1\rangle\rangle_\omega = \frac{1}{2\pi}\,\langle[\mathscr{C}_2, \mathscr{C}_1]\rangle + \langle\langle[\mathscr{C}_2, \mathscr{H}]; \mathscr{C}_1\rangle\rangle_\omega. \tag{3.2}$$

In our particular problem, this yields for $\langle\langle a_k^\dagger a_k; \mathscr{D}\rangle\rangle_{\omega+i\varepsilon}$:

$$(\omega + i\varepsilon)\,\langle\langle a_k^\dagger a_k; \mathscr{D}_\nu\rangle\rangle_{\omega+i\varepsilon} = \frac{1}{2\pi}\,\langle[a_k^\dagger a_k, \mathscr{D}_\nu]\rangle + \langle\langle[a_k^\dagger a_k, \mathscr{H}]; \mathscr{D}_\nu\rangle\rangle_{\omega+i\varepsilon} \tag{3.3}$$

with $\mathscr{H}$ given by (2.8). In virtue of the anticommutation rules for the fermion operators a_k, $a_k^\dagger$, the following relations hold:

$$\begin{aligned}[a_k^\dagger, \mathscr{H}] &= -E_k a_k^\dagger - \sum_q \lambda_q\, a_{k+q}^\dagger (b_q + b_{-q}^\dagger)\\ [a_k, \mathscr{H}] &= +E_k a_k + \sum_q \lambda_q\, a_{k-q}(b_q + b_{-q}^\dagger).\end{aligned} \tag{3.4}$$

Inserting (3.4) into (3.3), one obtains :

$$\begin{aligned}(\omega + i\varepsilon)\,\langle\langle a_k^\dagger a_k; \mathscr{D}_\nu\rangle\rangle_{\omega+i\varepsilon} &= \frac{1}{2\pi}\,\langle[a_k^\dagger a_k, \mathscr{D}_\nu]\rangle +\\ &+ \sum_q \lambda_q \langle\langle a_k^\dagger a_{k-q}(b_q + b_{-q}^\dagger); \mathscr{D}_\nu\rangle\rangle_{\omega+i\varepsilon} - \sum_q \lambda_q \langle\langle a_{k+q}^\dagger a_k (b_q + b_{-q}^\dagger); \mathscr{D}_\nu\rangle\rangle_{\omega+i\varepsilon}.\end{aligned} \tag{3.5}$$

By introducing the following definitions:

$$\begin{aligned}G_k(\omega + i\varepsilon) &= \langle\langle a_k^\dagger a_k; \mathscr{D}_\nu\rangle\rangle_{\omega+i\varepsilon}\\ G_{p_1, p_2}(\omega + i\varepsilon) &= \langle\langle a_{p_1}^\dagger a_{p_2} b_{p_1-p_2}; \mathscr{D}_\nu\rangle\rangle_{\omega+i\varepsilon}\\ G^{\perp}_{p_1, p_2}(\omega + i\varepsilon) &= \langle\langle a_{p_1}^\dagger a_{p_2} b_{p_2-p_1}^\dagger; \mathscr{D}_\nu\rangle\rangle_{\omega+i\varepsilon}{}^{*}),\end{aligned} \tag{3.6}$$

eq. (2.1) may be written as

$$\begin{aligned}(\omega + i\varepsilon)\, G_k(\omega + i\varepsilon) &= \frac{1}{2\pi}\,\langle[a_k^\dagger a_k, \mathscr{D}_\nu]\rangle + \sum_q \lambda_q [G_{k, k-q}(\omega+i\varepsilon) +\\ &+ G^{+}_{k, k-q}(\omega + i\varepsilon) - G_{k+q, k}(\omega + i\varepsilon) - G^{+}_{k+q, k}(\omega + i\varepsilon)].\end{aligned} \tag{3.7}$$

We remark that the Green's functions on the right hand side contain one

---

*) One has the relation $G^{+}_{p_1, p_2}(\omega + i\varepsilon) = -G^{*}_{p_2, p_1}(-\omega + i\varepsilon)$, where G^* denotes the complex conjugate of G.

b_q or $b^\dagger_{-q}$ more than the original Green's function $G_k(\omega + i\varepsilon)$. For each of these higher order Green's functions we may derive again an equation of motion as for instance

$$(\omega + i\varepsilon)\, G_{k,\,k-q}(\omega + i\varepsilon) =$$

$$= \frac{1}{2\pi} \langle [a^\dagger_k a_{k-q} b_q,\ \mathscr{D}_\nu] \rangle + \langle\langle [a^\dagger_k a_{k-q} b_q,\ \mathscr{H}];\ \mathscr{D}_\nu \rangle\rangle_{\omega + i\varepsilon}. \tag{3.8}$$

From the commutation rules of the Bose operators b_q and $b^\dagger_q$, it follows that

$$\begin{aligned} [b_q,\ \mathscr{H}] &= \omega_q b_q + \sum_k \lambda_q\, a^\dagger_{k-q} a_k \\ [b^\dagger_q,\ \mathscr{H}] &= -\omega_q b^\dagger_q - \sum_k \lambda_q a^\dagger_{b+q} a_k. \end{aligned} \tag{3.9}$$

By using (3.4) and (3.9), we get from eq. (3.7):

$$\begin{aligned} (\omega + i\varepsilon + E_k - E_{k-q} - \omega_q)\, G_{k,\,k-q}(\omega + i\varepsilon) = \frac{1}{2\pi} \langle [a^\dagger_k a_{k-q} b_q,\ \mathscr{D}_\nu] \rangle - \\ - \sum_{q_1} \lambda_{q_1} \langle\langle a^\dagger_{k+q_1} (b_{q_1} + b^\dagger_{-q_1}) a_{k-q} b_q;\ \mathscr{D}_\nu \rangle\rangle_{\omega + i\varepsilon} + \\ + \sum_{q_1} \lambda_{q_1} \langle\langle a^\dagger_k a_{k-q-q_1} (b_{q_1} + b^\dagger_{-q_1}) b_q;\ \mathscr{D}_\nu \rangle\rangle_{\omega + i\varepsilon} + \\ + \sum_{k'} \lambda_q \langle\langle a^\dagger_k a_{k-q} a^\dagger_{k'-q} a_{k'};\ \mathscr{D}_\nu \rangle\rangle_{\omega + i\varepsilon}. \end{aligned} \tag{3.10}$$

In an analoguous way we find

$$\begin{aligned} (\omega + i\varepsilon + E_k - E_{k-q} + \omega_q)\, G^+_{k,\,k-q}(\omega + i\varepsilon) = \frac{1}{2\pi} \langle [a^\dagger_k a_{k-q} b^\dagger_{-q},\ \mathscr{D}_\nu] \rangle - \\ - \sum_{q_1} \lambda_{q_1} \langle\langle a^\dagger_{k+q_1} (b_{q_1} + b^\dagger_{-q_1}) a_{k-q} b^\dagger_{-q};\ \mathscr{D}_\nu \rangle\rangle_{\omega + i\varepsilon} + \\ + \sum_{q_1} \lambda_{q_1} \langle\langle a^\dagger_k a_{k-q-q_1} (b_{q_1} + b^\dagger_{-q_1}) b^\dagger_{-q};\ \mathscr{D}_\nu \rangle\rangle_{\omega + i\varepsilon} - \\ - \sum_{k'} \lambda_q \langle\langle a^\dagger_k a_{k-q} a^\dagger_{k'-q} a_{k'};\ \mathscr{D}_\nu \rangle\rangle_{\omega + i\varepsilon}. \end{aligned} \tag{3.11}$$

By changing in (3.10) and (3.11) $k \to (k + q)$ and $(k - q) \to k$, we obtain directly the corresponding equations of motion for $G_{k+q,\,k}(\omega + i\varepsilon)$ and $G^+_{k+q,\,k}(\omega + i\varepsilon)$. Here again we have thus expressed the Green's functions on the left hand side by means of higher order Green's functions on the right hand side. Now we could go further and write the latter Green's function again in terms of higher order ones and so on; generally speaking we would obtain a chain of coupled integral equations, each Green's function of order n being expressed by means of Green's function of order $n + 1$ (n being the total number of creation and annihilation operators on the left hand side of the Green's function). In order to deal with this chain

of equations one has to establish an expression of the higher order Green's functions in terms of the lower order ones.

4. *Derivation of the kinetic equations.* Following a method also used in the article of Zubarev[7]), we break off the chain of equations by decoupling, i.e. we express in a well defined way the n-th order Green's functions in terms of lower order ones. This decoupling process is of course an approximation the meaning of which is not immediately transparent. It becomes more clear by the following reasoning. As already remarked, $\langle\langle a_k^\dagger a_k;\ \mathscr{D}_v\rangle\rangle_{\omega+i\varepsilon}$ is the linear correction (due to the electric field) to the equilibrium value of the electron density $\langle a_k^\dagger a_k\rangle = n_k$. Similarly, the Green's function $\langle\langle a_{k+q_1}^\dagger a_{k-q} b_{-q_1}^\dagger b_q;\ \mathscr{D}_v\rangle\rangle_{\omega+i\varepsilon}$ is the correction to the equilibrium value of the more complicated distribution function $\langle a_{k+q_1}^\dagger a_{k-q} b_{-q_1}^\dagger b_q\rangle$. This higher order distribution function may be written as

$$\langle a_{k+q_1}^\dagger a_{k-q} b_{-q_1}^\dagger b_q\rangle = \langle a_{k+q_1}^\dagger a_{k-q}\rangle \langle b_{-q_1}^\dagger b_q\rangle + \text{correction terms}, \qquad (4.1)$$

where the correction terms are of higher order in the electron phonon coupling λ_q. Now perturbing (4.1) by an electric field $\boldsymbol{E}\exp(-i\omega t + \varepsilon t)$, we obtain in lowest order in $\boldsymbol{E}$ for the deviation caused by $\boldsymbol{E}$:

$$\begin{aligned}
&\langle\langle a_{k+q_1}^\dagger a_{k-q} b_{-q_1}^\dagger b_q;\ \mathscr{D}_v\rangle\rangle_{\omega+i\varepsilon} = \\
&= \langle\langle a_{k+q_1}^\dagger a_{k-q};\ \mathscr{D}_v\rangle\rangle_{\omega+i\varepsilon} \langle b_{-q_1}^\dagger b_q\rangle + \langle a_{k+q_1}^\dagger a_{k-q}\rangle \langle\langle b_{-q_1}^\dagger b_q;\ \mathscr{D}_v\rangle\rangle + \ldots = \\
&= \delta_{q+q_1}\{\langle\langle a_{k-q}^\dagger a_{k-q};\ \mathscr{D}_v\rangle\rangle_{\omega+i\varepsilon} v_q + n_{k-q}\langle\langle b_q^\dagger b_q;\ \mathscr{D}_v\rangle\rangle_{\omega+i\varepsilon}\} + \ldots \qquad (4.2)
\end{aligned}$$

The first term is the contribution due to the perturbation of the electron distribution at a constant phonon distribution v_q, while the second term is the contribution due to the perturbation of the phonon distribution at a constant electron distribution n_{k-q}. The correction term may be discussed by decoupling in a higher order stage of the hierarchy as will be done in the next chapter. We note that also the terms with bb or $b^\dagger b^\dagger$ as for instance $\langle\langle a_{k+q_1}^\dagger b_{q_1} a_{k-q} b_q;\ \mathscr{D}_v\rangle\rangle_{\omega+i\varepsilon}$ are of higher order in the electron phonon coupling λ_q. In the order considered here, they may be omitted. So in lowest order we have to consider only Green's functions in which the a's and b's can be grouped into pairs of a creation and an annihilation operator i.e. $a^\dagger a$ and $b^\dagger b$.

The last Green's function on the right hand side of eq. (3.10) contains four fermion operators, the corresponding distribution function $\langle a_k^\dagger a_{k-q} a_{k'-q}^\dagger a_{k'}\rangle$ may be written as:

$$\langle a_k^\dagger a_{k-q}\, a_{k'-q}^\dagger a_{k'}\rangle = \delta_{q+0}\langle a_k^\dagger a_k\rangle \langle a_{k'}^\dagger a_{k'}\rangle + \delta_{k-k'}\langle a_k^\dagger a_k\rangle\langle a_{k-q} a_{k-q}^\dagger\rangle + \ldots \qquad (4.3)$$

Here the first term of the right hand side is zero except for $q = 0$. In this case however the factor λ_q in eq. (3.10) which stands in front of the corresponding Green's function is zero, and thus the first term of the right hand

side of (4.3) does not contribute. Therefore we have to consider only the deviation from equilibrium of the second term of the right hand side of eq. (4.3) and this may be written as:

$$\ll a_k^\dagger a_{k-q} a_{k'-q}^\dagger a_{k'};\ \mathscr{D}_\nu \gg_{\omega+i\varepsilon} =$$
$$= \delta_{k-k'}\{(1-n_{k-q})\ \ll a_k^\dagger a_k;\ \mathscr{D}_\nu \gg_{\omega+i\varepsilon} - n_k \ll a_{k-q}^\dagger a_{k-q};\ \mathscr{D}_\nu \gg_{\omega+i\varepsilon}\}. \qquad (4.5)$$

With the use of eq. (4.2), and (4.4), eq. (3.10) becomes

$$(\omega + i\varepsilon + E_k - E_{k-q} - \omega_q)\ \boldsymbol{G}_{k,\,k-q}(\omega + i\varepsilon) = \frac{1}{2\pi} \langle [a_k^\dagger a_{k-q} b_q,\ \mathscr{D}_\nu] \rangle -$$
$$- \lambda_q \{(\nu_q + n_k)\ \boldsymbol{G}_{k-q}(\omega + i\varepsilon) - (1 + \nu_q - n_{k-q})\ \boldsymbol{G}_k(\omega + i\varepsilon) -$$
$$- (n_k - n_{k-q})\ \boldsymbol{D}_q(\omega + i\varepsilon)\} \qquad (4.5)$$

where $\boldsymbol{D}_q(\omega + i\varepsilon)$ is defined by

$$\boldsymbol{D}_q(\omega + i\varepsilon) = \ll b_q^\dagger b_q;\ \mathscr{D}_\nu \gg_{\omega+i\varepsilon}. \qquad (4.6)$$

In the similar way, eq. (3.11) is found to be

$$(\omega + i\varepsilon + E_k - E_{k-q} + \omega_q)\ \boldsymbol{G}^+_{k,\,k-q}(\omega + i\varepsilon) = \frac{1}{2\pi} \langle [a_k^\dagger a_{k-q} b_{-q},\ \mathscr{D}_\nu] \rangle -$$
$$- \lambda_q \{(1 + \nu_q - n_k)\ \boldsymbol{G}_{k-q}(\omega + i\varepsilon) - (\nu_q + n_{k-q})\ \boldsymbol{G}_k(\omega + i\varepsilon) -$$
$$- (n_k - n_{k-q})\ \boldsymbol{D}_{-q}(\omega + i\varepsilon)\} \qquad (4.7)$$

With respect to the Green's functions $\boldsymbol{G}_{k+q,\,k}(\omega + i\varepsilon)$ and $\boldsymbol{G}^+_{k+q,\,k}(\omega + i\varepsilon)$ we remark that if a Green's function transforms into another one by changing $k \to (k \mp q)$ and $(k - q) \to k$, their expressions, obtained from the decoupling approximation, transform also into each other by the same change of variables. Thus from eqs. (4.5) and (4.7) we obtain immediately by changing $k \to (k + q)$ and $(k - q) \to k$ the corresponding equations for $\boldsymbol{G}_{k+q,\,k}(\omega + i\varepsilon)$ and $\boldsymbol{G}^+_{k+q,\,k}(\omega + i\varepsilon)$.

Now all higher order Green's functions which occur in the right hand side of eq. (3.8) are replaced by the expressions obtained from eqs. (4.5), (4.7) and thus we get an equation which contains only $\boldsymbol{G}_k(\omega + i\varepsilon)$ and $\boldsymbol{D}_q(\omega + i\varepsilon)$:

$$(\omega + i\varepsilon)\ \boldsymbol{G}_k(\omega + i\varepsilon) = + \frac{i}{2\pi} \frac{\partial n_k}{\partial k_\nu} + \sum_q \{[W^{(1)}_{k,\,k+q}(\omega + i\varepsilon) +$$
$$+ W^{(2)}_{k,\,k+q}(\omega + i\varepsilon)]\ \boldsymbol{G}_k(\omega \mp i\varepsilon) - [W^{(1)}_{k+q,\,k}(\omega + i\varepsilon) +$$
$$+ W^{(2)}_{k+q,\,k}(\omega + i\varepsilon)]\ \boldsymbol{G}_{k+q}(\omega + i\varepsilon) +$$
$$+ W^{(3)}_{k,\,k+q}(\omega + i\varepsilon)\ \boldsymbol{D}_{-q}(\omega + i\varepsilon) - W^{(3)}_{k+q,\,k}(\omega + i\varepsilon)\ \boldsymbol{D}_q(\omega + i\varepsilon)\}. \qquad (4.8)$$

Here the first term on the right hand side comes from

$$\langle [a_k^\dagger a_k,\ \mathscr{D}_\nu] \rangle = \frac{i\partial n_k}{\partial k_\nu}, \tag{4.9}$$

a result which is proved by elementary quantum mechanics. The quantities $W^{(1)}$, $W^{(2)}$ and $W^{(3)}$ are defined by ($q = k_1 - k_2$):

$$W^{(1)}_{k_1, k_2}(\omega) = \lambda_q^2(1 + \nu_q - n_{k_2})\ \mathrm{d}(E_{k_1} - E_{k_2} - \omega_q, \omega) \tag{4.10}$$

$$W^{(2)}_{k_1, k_2}(\omega) = \lambda_q^2(\nu_q + n_{k_2})\ \mathrm{d}(E_{k_2} - E_{k_1} - \omega_q, \omega) \tag{4.11}$$

$$W^{(3)}_{k_1, k_2}(\omega) = \lambda_q^2(n_{k_1} - n_{k_2})\ \mathrm{d}(E_{k_1} - E_{k_2} - \omega_q, \omega) \tag{4.12}$$

where $\mathrm{d}(X, \omega)$ is given by

$$\mathrm{d}(X, \omega) = \frac{1}{X + \omega} - \frac{1}{X - \omega}. \tag{4.13}$$

For $\omega = i\varepsilon$, the last relation reduces to a δ-function representation:

$$\mathrm{d}(X, i\varepsilon) = \frac{1}{X + i\varepsilon} - \frac{1}{X - i\varepsilon} = -2\pi i\ \delta(X). \tag{4.14}$$

In eq. (4.8), the quantities $W^{(i)}$, ($i = 1, 2, 3$) are of second order in λ_q. This follows from the fact that we did already break off the chain in eqs. (3.10), (3.11). If we had developed our system of equations of motion further, we would be led to decouple Green's functions of higher order than those occurring in eqs. (3.10), (3.11). Their decoupling would give again the result we did obtain, plus additional terms which are of order λ_q^4, λ_q^6, ... etc.

We remark also that we did not take into account contributions arising from terms like $\langle [a_k^\dagger a_{k-q} b_q,\ \mathscr{D}_\nu] \rangle$ i.e. the commutators, on the right hand side, of eqs. (4.5), (4.7). We shall show in the following chapter that these contributions are of higher order in λ_q and therefore corrections to $\partial n_k / \partial k_\nu$. Thus it is clear that eq. (4.8) is an approximation, correct only in lowest order i.e. λ_q^2, but at this stage the functions $\boldsymbol{D}_q(\omega + i\varepsilon)$ are already present. These contributions come from the last terms on the right hand side of eq. (4.2), they are due to the perturbation of the phonon distribution function.

Let us now examine the function $\boldsymbol{D}_q(\omega + i\varepsilon)$ in more detail. From the equation of motion (3.2) and the commutation relations (3.9), we get

$$(\omega + i\varepsilon)\ \boldsymbol{D}_q(\omega + i\varepsilon) = 0 - \sum_k \lambda_q\, \boldsymbol{G}_{k+q,\,k}(\omega + i\varepsilon) + \sum_k \lambda_q\, \boldsymbol{G}^+_{k-q,\,k}(\omega + i\varepsilon). \tag{4.15}$$

The equations for $\boldsymbol{G}_{k+q,\,k}(\omega + i\varepsilon)$ and $\boldsymbol{G}^+_{k-q,\,k}(\omega + i\varepsilon)$ are of the same type as eqs. (4.5), (4.7) and may be obtained from the latter by changing the arguments. Inserting the values thus obtained for $\boldsymbol{G}_{k+q,\,k}(\omega + i\varepsilon)$ and

$G^+_{k-q,\,k}(\omega + i\varepsilon)$ into eq. (4.15), yields

$$(\omega + i\varepsilon)\, \boldsymbol{D}_q(\omega + i\varepsilon) =$$

$$\sum_k \left[\frac{\lambda_q^2}{\omega + E_{k+q} - E_k - \omega_q + i\varepsilon} \right] \cdot$$

$$\cdot [(v_q + n_{k+q}) \boldsymbol{G}_k(\omega + i\varepsilon) - (1 + v_q - n_k) \boldsymbol{G}_{k-q}(\omega + i\varepsilon) - (n_{k+q} - n_k) \boldsymbol{D}_q(\omega + i\varepsilon)] +$$

$$+ \sum_k \left[\frac{\lambda_q^2}{\omega + E_{k-q} - E_k + \omega_q + i\varepsilon} \right] \cdot$$

$$\cdot [(v_q + n_k) \boldsymbol{G}_{k-q}(\omega + i\varepsilon) - (1 + v_q - n_{k-q}) \boldsymbol{G}_k(\omega + i\varepsilon) - (n_k - n_{k-q}) \boldsymbol{D}_q(\omega + i\varepsilon).] \tag{4.16}$$

This equation has been obtained under the same conditions as eq. (4.8). By replacing in the last sum $(k-q)$ by k and k by $(k + q)$, eq. (4.16) may be written as:

$$(\omega + i\varepsilon)\, \boldsymbol{D}_q(\omega + i\varepsilon) = \sum_k \{ W^{(2)}_{k,\,k-q}(\omega + i\varepsilon)\, \boldsymbol{G}_k(\omega + i\varepsilon) -$$

$$W^{(1)}_{k+q,\,k}(\omega + i\varepsilon)\, \boldsymbol{G}_{k+q}(\omega + i\varepsilon) - W^{(3)}_{k+q,\,k}(\omega + i\varepsilon) \boldsymbol{D}_q(\omega + i\varepsilon) \} \tag{4.17}$$

Eq. (4.8) together with (4.17) constitutes a set of two coupled linear integral equations for the deviations from equilibrium $\boldsymbol{G}_k$ and $\boldsymbol{D}_q$ of the electron and the phonon distribution. By the two last terms of the right hand side of (4.8) and the two first terms of the right hand side of (4.17) the deviations $\boldsymbol{G}_k$ and $\boldsymbol{D}_q$ are coupled to each other. Therefore they are also of the same order in the coupling for $\omega = 0$ i.e. of order λ_q^{-2}. For $\omega = 0$, both the left hand sides of (4.8) and (4.17) vanish and so in (4.8) $\boldsymbol{G}_k$ (and/or $\boldsymbol{D}_q$) has to be of order λ_q^{-2} in order to compensate $\partial n_k / \partial k$ which is of order λ_q^0. Then it follows from (4.17) that also $\boldsymbol{D}_q(\boldsymbol{G}_k)$ is of order λ_q^{-2}. Thus the occurrence of the two last terms on the right hand side of (4.8) is for $\omega = 0$ not an higher order effect; they have to be taken into account for the evaluation of the static electrical conductivity in the lowest order in the coupling.

A posteriori this is the reason that we have retained only the Green's functions $\boldsymbol{G}_k$ and $\boldsymbol{D}_q$ in the decoupling process and dropped out all other Green's functions as for instance $\langle\langle b_q b_{-q};\, \boldsymbol{D}_\nu \rangle\rangle_\omega$. In the equation of motion for $\langle\langle b_q b_{-q};\, \boldsymbol{D}_\nu \rangle\rangle_\omega$ the left hand side does not vanish for $\omega = 0$ (since $b_q b_{-q}$ does not commute with the free Hamiltonian, like $a_k^\dagger a_k$ and $b_q^\dagger b_q$ do) and this shows that $\langle\langle b_q b_{-q};\, \mathscr{D}_\nu \rangle\rangle$ is of order λ_q^0 for $\omega = 0$.

For $\omega = 0$ we can compare equations (4.8) and (4.17) with the usual Boltzmann equations for the electron and the phonon distribution functions f^e and f^p. For a stationary state in a static electric field, the Boltzmann

equations may be written as:

$$0 = \left(\frac{\partial f^e}{\partial t}\right)_{\text{coll.}} + \left(\frac{\partial f^e}{\partial t}\right)_{\text{str.}}$$
$$0 = \left(\frac{\mathrm{d} f^p}{\partial t}\right)_{\text{coll.}} \tag{4.18}$$

where the collision and the streaming rates of change read[8)9)] (in our notation and without spin):

$$\left(\frac{\partial f^e}{\partial t}\right)_{\text{str.}} = -\, e\, \boldsymbol{E}.\, \frac{\partial f^e_k}{\partial k}$$

$$\left(\frac{\partial f^e}{\partial t}\right)_{\text{coll.}} = \sum_q 2\pi\, \lambda_q^2\, \delta(E_{k+q} - E_k - \omega_q)\, [(1 + f^p_q) f^e_{k+q}(1 - f^e_k) - f^p_q\, f^e_k (1 - f^e_{k+q})] -$$
$$- \sum_q 2\pi\, \lambda_q^2\, \delta(E_{k+q} - E_k + \omega_q) [(1 + f^p_{-q})\, f^e_k (1 - f^e_{k+q}) - f^p_{-q} f^e_{k+q} (1 - f^e_k)],$$

$$\left(\frac{\partial f^p}{\partial t}\right)_{\text{coll.}} = \sum_k 2\pi\, \lambda_q^2\, \delta(E_{k+q} - E_k - \omega_q)\, [(1 + f^p_q) f^e_{k+q}(1 - f^e_k) - f^p_q f^e_k (1 - f^e_{k+q})]. \tag{4.19}$$

According to eq. (2.15) we have the relations:

$$f^e_k = n_k - 2\pi e\, \boldsymbol{E} \cdot \boldsymbol{G}_k,$$
$$f^p_q = \nu_q - 2\pi e\, \boldsymbol{E} \cdot \boldsymbol{D}_q, \tag{4.20}$$

within the terms linear in the electric field. Inserting (4.20) and (4.19) into (4.18) and collecting the terms proportional to the electric field $\boldsymbol{E}$, exactly gives equations (4.8) and (4.17) for $\omega = 0$. Thus (4.8) and (4.17) are the Boltzmann equations for the electron and phonon distribution induced by the electric field and the electron-phonon coupling (phonon drag). The latter has not been taken into account by Fujita[3]). Even in the case of low electron density n_k this phonon drag persists in lowest order in λ_q although the coupling between $\boldsymbol{G}_k$ and $\boldsymbol{D}_q$ is proportional to n_k in (4.8). When solving $\boldsymbol{D}_q$ with respect to $\boldsymbol{G}_k$ from (4.17) (as is possible in this order)

$$\boldsymbol{D}_q(\omega + i\varepsilon) =$$
$$= \frac{\sum_k [W^{(2)}_{k,\,k+q}(\omega + i\varepsilon)\; \boldsymbol{G}_k(\omega + i\varepsilon) - W^{(1)}_{k+q,\,k}(\omega + i\varepsilon)\; \boldsymbol{G}_{k+q}(\omega + i\varepsilon)]}{\omega + i\varepsilon + \sum_k W^{(3)}_{k+q,\,k}(\omega + i\varepsilon)} \tag{4.21}$$

it follows for $\omega = 0$ that $\boldsymbol{D}_q$ is proportional to $(n_k)^{-1}$ and thus even for small n_k the two last terms (phonon drag) on the right hand side in (4.8) may not be neglected as has been done by Zubarev[7]).

In this case of static field, the occurrence of phonon drag has very drastic

consequences: if one neglects "Umklapprozesse" (as is done in this section), the static electrical conductivity becomes infinite, as shall be outlined in the next section. This follows from the fact that for $\omega = 0$, the set of coupled integral equations (4.8) and (4.17) has no finite solution $\boldsymbol{G}_k$.

5. *Conservation laws.* Generally speaking, let us suppose that the operator $\mathscr{C}_2$ which we considered in section 2 commutes with the Hamiltonian $\mathscr{H}$ of the unperturbed system, in other words, the physical quantity corresponding to $\mathscr{C}_2$ is conserved in absence of external perturbation. Then the Green's function $\langle\langle \mathscr{C}_2; \mathscr{C}_1 \rangle\rangle_t$ defined by (2.4) becomes

$$\langle\langle \mathscr{C}_2; \mathscr{C}_1 \rangle\rangle_t = -i\theta(t) \langle [\mathscr{C}_2(0), \mathscr{C}_1(0)] \rangle \tag{5.1}$$

and eq. (2.6) may be written as

$$\Delta \langle \mathscr{C}_2 \rangle_{t'=0} = -2\pi A \langle\langle \mathscr{C}_2; \mathscr{C}_1 \rangle\rangle_{\omega+i\varepsilon} = \frac{A \langle [\mathscr{C}_2, \mathscr{C}_1] \rangle}{\omega + i\varepsilon}. \tag{5.2}$$

Formula (5.2) shows that the linear response of a quantity which is conserved in the absence of an external field becomes infinite for $\omega = 0$ unless the average value of the commutator i.e. $\langle [\mathscr{C}_2, \mathscr{C}_1] \rangle$ vanishes.

With respect to our particular problem when the unperturbed system is described by the Fröhlich Hamiltonian (2.8), while $\Delta\mathscr{H}$ is given by eq. (2.9), we have the following conserved quantities:

$$\begin{aligned} \mathscr{N} &= \sum_k a_k^\dagger a_k \\ \mathscr{P} &= \sum_k \boldsymbol{k} a_k^\dagger a_k + \sum_q \boldsymbol{q} b_q^\dagger b_q \\ \mathscr{H} &= \sum_k E_k a_k^\dagger a_k + \sum_q \omega_q b_q^\dagger b_q + \sum_{k,q} \lambda_q a_k^\dagger a_{k-q} (b_q + b_{-q}^\dagger) \end{aligned} \tag{5.3}$$

referring to the number of electrons, the total (quasi-) momentum of the electron-phonon system and the total energy of the system. As regards the conservation of the total momentum, one has to neglect the so called "Umklapprozesse" as we did in the foregoing. For the averages of the commutators of these conserved quantities with the totale dipole moment $\mathscr{D}$ ($\mathscr{D}$ plays the role of $\mathscr{C}_1$) of the system, one finds

$$\begin{aligned} \langle [\mathscr{N}, \mathscr{D}] \rangle &= \langle 0 \rangle = 0 \\ \langle [\mathscr{P}, \mathscr{D}] \rangle &= i \langle \mathscr{N} I \rangle = + iNI, \; (I_{\mu\nu} = \delta_{\mu\nu}) \\ \langle [\mathscr{H}, \mathscr{D}] \rangle &= i \langle \dot{\mathscr{D}} \rangle = \frac{i}{m} \sum_k \boldsymbol{k} \langle a_k^\dagger a_k \rangle = 0 \end{aligned} \tag{5.4}$$

where m is the one electron mass and N the total electron number.

So one observes that the linear response for the number of electrons and the total energy is zero while the linear response of the total quasi momen-

tum reads

$$\Delta\langle \mathscr{P} \rangle = -2\pi e \, \boldsymbol{E} \, \langle\!\langle \mathscr{P}; \mathscr{D} \rangle\!\rangle_{\omega + i\varepsilon} = \frac{ieN\boldsymbol{E}}{\omega + i\varepsilon}, \tag{5.5}$$

which becomes infinite for $\omega \to 0$.

The conservation laws may also be formulated in terms of the Green's functions $\boldsymbol{G}_k(\omega + i\varepsilon)$, $\boldsymbol{D}_q(\omega + i\varepsilon)$ and $\boldsymbol{G}_{k,k'}(\omega + i\varepsilon)$ defined in eqs. (3.6) and (4.6). By inserting expressions (5.3) into (5.2) where $\mathscr{C}_1 = \mathscr{D}$, we obtain the following relations

$$\sum_k \boldsymbol{G}_k(\omega + i\varepsilon) = 0,$$

$$-2\pi(\omega + i\varepsilon)\left[\sum_k \boldsymbol{k}\boldsymbol{G}_k(\omega + i\varepsilon) + \sum_q \boldsymbol{q}\boldsymbol{D}_q(\omega + i\varepsilon)\right] = iNI, \tag{5.6}$$

$$\sum_k E_k \boldsymbol{G}_k(\omega + i\varepsilon) + \sum_q \omega_q \boldsymbol{D}_q(\omega + i\varepsilon) + \sum_{k,q} \lambda_q [\boldsymbol{G}_{k,k+q}(\omega + i\varepsilon) + \boldsymbol{G}^{+}_{k,k+q}(\omega + i\varepsilon)] = 0.$$

So it follows that for $\omega \to 0$, either $\sum_k \boldsymbol{k}\boldsymbol{G}_k(\omega + i\varepsilon)$ or $\sum_q \boldsymbol{q}\boldsymbol{D}_q(\omega + i\varepsilon)$ must tend to infinity or both. But inspecting the kinetic equations (4.8) and (4.17) one concludes that both $\sum_k \boldsymbol{G}(\omega + i\varepsilon)$ and $\sum_q \boldsymbol{q}\boldsymbol{D}_q(\omega + i\varepsilon)$ must tend to infinity for $\omega \to 0$ because they are interrelated by the phonon drag terms.

It should be stressed that the relations (5.6) which were derived from the conservation laws (5.4), also follow from the kinetic equations, i.e. in the kinetic equations, the conservation laws are included. For the exact kinetic equations (i.e. to any order) this is obvious. However it turns out to be the case also for the approximate kinetic equations (4.8) and (4.17) which were derived in section 4 by the decoupling technique.

The conservation of the number of electrons is merely a consequence of the symmetry between $\boldsymbol{G}^{(+)}_{k,k-q}(\omega + i\varepsilon)$ and $\boldsymbol{G}^{(+)}_{k+q,k}(\omega + i\varepsilon)$ in (3.7) as one sees from summing (3.7) over k and changing $(k + q) \to k$ for the two last terms. As already stated, this symmetry remains also after the decoupling process.

The conservation of total momentum results from the same symmetry in (3.7) and the changes of variables together with the use of eq. (4.15).

The conservation of energy follows from the same properties of (3.7) and (4.15) in addition with the relation

$$\sum_k (\omega + i\varepsilon + E_k - E_{k-q} - \omega_q)\, \boldsymbol{G}_{k,k-q}(\omega + i\varepsilon) + \sum_k (\omega + i\varepsilon + E_k - E_{k-q} + \omega_q) \cdot$$

$$\boldsymbol{G}_{k,k-q}(\omega + i\varepsilon) = \frac{1}{2\pi} \sum_k \langle [(a^{\dagger}_k a_{k-q} b_q + a^{\dagger}_k a_{k-q} b^{\dagger}_{-q}),\, \mathscr{D}_v] \rangle = 0 \tag{5.7}$$

which is obtained by adding eqs. (3.10) and (3.11) and which clearly also holds after decoupling of the right hand side terms of eqs. (3.10) and (3.11).

Moreover, for $\omega = 0$ one has in lowest order the conservation law:

$$\sum_k E_k G_k(i\varepsilon) + \sum_q \omega_q D_q(i\varepsilon) = 0 \tag{5.8}$$

since the last two terms in the last equation of (5.6) are of higher order in λ_q. One verifies that (5.8) also follows from the lowest order Boltzmann equations (4.8) and (4.17) (for $\omega = 0$).

6. *Umklapprozesse.* All calculations of the foregoing sections 3, 4 have been made with the use of the Hamiltonian (2.8), the interaction term of which describes only "Normalprozesse". In the present section we give the derivation of the kinetic equations including Umklapprozesse. The Hamiltonian of the electron-phonon-system reads now:

$$\mathscr{H}^u = \sum_k E_k\, a_k^\dagger a_k + \sum_q \omega_q b_q^\dagger b_q + \sum_{q,k,g} \lambda_q\, a_{k+q+g}^\dagger\, a_k (b_q + b_{-q}^\dagger) \tag{6.1}$$

where the sum over g runs over the reciprocal lattice. For $g = 0$, (6.1) reduces to (2.8). (In (6.1) we do not consider explicitly the phonon polarisations but a summation thereover does not introduce any essential change of our formalism).

We briefly sketch the different steps of the calculation. Instead of (3.5) one gets the following equation of motion for the Green's function $\langle\langle a_k^\dagger a_k;\ \mathscr{D}_\nu\rangle\rangle_{\omega+i\varepsilon}$:

$$\begin{aligned}(\omega + i\varepsilon)\,\langle\langle a_k^\dagger a_k;\ \mathscr{D}_\nu\rangle\rangle_{\omega+i\varepsilon} = {} & \frac{1}{2\pi}\langle[a_k^\dagger a_k,\ \mathscr{D}_\nu]\rangle + \\ & + \sum_{q,g} \lambda_q\,\langle\langle a_k^\dagger a_{k-q-g}(b_q + b_{-q}^\dagger);\ \mathscr{D}_\nu\rangle\rangle_{\omega+i\varepsilon} - \\ & - \sum_{q,g} \lambda_q\,\langle\langle a_{k+q+g}^\dagger a_k (b_q + b_{-q}^\dagger);\ \mathscr{D}_\nu\rangle\rangle_{\omega-i\varepsilon}.\end{aligned} \tag{6.2}$$

The equations of motion of the higher order Green's functions have also to be modified, e.g. (3.11) becomes:

$$\begin{aligned}(\omega + i\varepsilon + E_k - E_{k-q-g} - \omega_q)\,\langle\langle a_k^\dagger a_{k-q-g} b_q;\ \mathscr{D}_\nu\rangle\rangle_{\omega+i\varepsilon} = {} & \frac{1}{2\pi}\langle[a_k^\dagger a_{k-q-g} b_q,\ \mathscr{D}_\nu]\rangle + \\ & + \sum_{q_1,g'} \lambda_{q_1}\,\langle\langle a_k^\dagger a_{k-q-g-q_1-g'}(b_{q_1} + b_{-q_1}^\dagger) b_q;\ \mathscr{D}_\nu\rangle\rangle_{\omega+i\varepsilon} - \\ & - \sum_{q_1,g'} \lambda_{q_1}\,\langle\langle a_{k+q_1+g'}^\dagger (b_{q_1} + b_{-q_1}^\dagger) a_{k-q-g} b_q;\ \mathscr{D}_\nu\rangle\rangle_{\omega+i\varepsilon} + \\ & + \sum_{k',g'} \lambda_q\,\langle\langle a_k^\dagger a_{k-q-g} a_{k'}^\dagger a_{k'+q+g'};\ \mathscr{D}_\nu\rangle\rangle_{\omega+i\varepsilon}.\end{aligned} \tag{6.3}$$

The higher order Green's functions on the right hand side of eq. (6.3) are

decoupled as follows:

$$\sum_{q_1 g'} \lambda_{q_1} \langle\langle a^\dagger_{k+q_1+g'} b^\dagger_{-q_1} b_q \, a_{k-q-g}; \mathscr{D}_\nu \rangle\rangle =$$

$$= \lambda_q [\nu_q \sum_{g'} \langle\langle a^\dagger_{k-q+g'} a_{k-q-g}; \mathscr{D}_\nu \rangle\rangle + \sum_{g'} \langle a^\dagger_{k-q+g'} a_{k-q-g} \rangle \langle\langle b^\dagger_q b_q; \mathscr{D}_\nu \rangle\rangle] =$$

$$= \lambda_q [\nu_q \langle\langle a^\dagger_{k-q-g} a_{k-q-g}; \mathscr{D}_\nu \rangle\rangle + n_{k-q-g} \langle\langle b^\dagger_q b_q; \mathscr{D}_\nu \rangle\rangle] +$$

$$+ \text{ terms of higher order in } \lambda_q. \tag{6.4}$$

Here we did use the fact that $\langle\langle a^\dagger_{k-q+g'} a_{k-q-g}; \mathscr{D}_\nu \rangle\rangle$, $\langle a^\dagger_{k-q+g'} a_{k-q-g} \rangle$ with $g' \neq -g$ are of higher order in λ_q compared to $\langle\langle a^\dagger_{k-q-g} a_{k-q-g}; \mathscr{D}_\nu \rangle\rangle$, $\langle a^\dagger_{k-q-g} a_{k-q-g} \rangle$. This follows directly from the fact that for $\omega = 0$, the left hand side term of the equation of motion for $\langle\langle a^\dagger_{k-q-g} a_{k-q-g}; \mathscr{D}_\nu \rangle\rangle$ vanishes while this is not the case for $\langle\langle a^\dagger_{k-q+g'} a_{k-q-g}; \mathscr{D}_\nu \rangle\rangle$ (cf. also sect. 4). Decoupling in a similar way also the other Green's functions on the right hand side of (6.3), one obtains in lowest order in λ_q:

$$(\omega + i\varepsilon + E_k - E_{k-q-g} - \omega_q) \langle\langle a^\dagger_k a_{k-q-g} b_q; \mathscr{D}_\nu \rangle\rangle_{\omega + i\varepsilon} =$$

$$= \frac{1}{2\pi} \langle [a^\dagger_k a_{k-q-g} b_q, \mathscr{D}_\nu] \rangle - \lambda_q (\nu_q + n_k) \, \boldsymbol{G}_{k-q-g} +$$

$$+ \lambda_q (1 + \nu_q - n_{k-q-g}) \boldsymbol{G}_k - \lambda_q \, (n_{k-q-g} - n_k) \, \boldsymbol{D}_q. \tag{6.5}$$

A similar equation is found for $\langle\langle a^\dagger_k a_{k-q-g} b^\dagger_{-q}; \mathscr{D}_\nu \rangle\rangle_{\omega + i\varepsilon}$:

$$(\omega + i\varepsilon + E_k - E_{k-q-g} + \omega_q) \, \langle\langle a^\dagger_k a_{k-q-g} b^\dagger_{-q}; \mathscr{D}_\nu \rangle\rangle_{\omega + i\varepsilon} =$$

$$= \frac{1}{2\pi} \langle [a^\dagger_k a_{k-q-g} b^\dagger_{-q}, \mathscr{D}_\nu] \rangle - \lambda_q (1 + \nu_q - n_k) \, \boldsymbol{G}_{k-q-g} +$$

$$+ \lambda_q (\nu_q + n_{k-q-g}) \boldsymbol{G}_k - \lambda_q (n_{k-q-g} - n_k) \, \boldsymbol{D}_{-q}. \tag{6.6}$$

By using (6.5), (6.6) and by remarking the symmetry between the Green's functions of the right hand side of eq. (6.2), one finds in lowest order in λ_q:

$$(\omega + i\varepsilon) \, \boldsymbol{G}_k(\omega + i\varepsilon) = \frac{i}{2\pi} \frac{\partial n_k}{\partial k_\nu} +$$

$$+ \sum_{q, g} \{ [W^{(1)}_{k, k+q+g}(\omega + i\varepsilon) + W^{(2)}_{k, k+q+g}(\omega + i\varepsilon)] \boldsymbol{G}_k(\omega + i\varepsilon) -$$

$$- [W^{(1)}_{k+q+g, k}(\omega + i\varepsilon) + W^{(2)}_{k+q+g, k}(\omega + i\varepsilon)] \, \boldsymbol{G}_{k+q+g, k}(\omega + i\varepsilon) +$$

$$+ W^{(3)}_{k, k+q+g}(\omega + i\varepsilon) \, \boldsymbol{D}_{-q}(\omega + i\varepsilon) - W^{(3)}_{k+q+g, k}(\omega + i\varepsilon) \, \boldsymbol{D}_q(\omega + i\varepsilon) \} \tag{6.7}$$

where $W^{(1)}$, $W^{(2)}$, $W^{(3)}$ are again defined by (4.10) — (4.12). Similarly the equation of motion for $\langle\langle b^\dagger_q b_q; \mathscr{D}_\nu \rangle\rangle_{\omega + i\varepsilon} = \boldsymbol{D}_q(\omega + i\varepsilon)$is given by

$$(\omega + i\varepsilon) \, \boldsymbol{D}_q(\omega + i\varepsilon) = - \sum_{k, g} \lambda_q \, \langle\langle a^\dagger_{k+q+g} a_k b_q; \mathscr{D}_\nu \rangle\rangle_{\omega + i\varepsilon} +$$

$$+ \sum_{k, g} \lambda_q \, \langle\langle b^\dagger_q a^\dagger_k a_{k+q+g}; \mathscr{D}_\nu \rangle\rangle_{\omega + i\varepsilon}, \tag{6.8}$$

from which the kinetic equation in lowest order in λ_q is found to be:

$$(\omega + i\varepsilon)\, \boldsymbol{D}_q(\omega + i\varepsilon) = \sum_{k,\, g} \{W^{(2)}_{k,\, k+q+g}(\omega + i\varepsilon)\boldsymbol{G}_k(\omega + i\varepsilon) -$$

$$- W^{(1)}_{k+q+g,\, k}(\omega + i\varepsilon)\boldsymbol{G}_{k+q+g}(\omega + i\varepsilon) - W^{(3)}_{k+q+g,\, k}(\omega + i\varepsilon)\, \boldsymbol{D}_q(\omega + i\varepsilon)\} \quad (6.9)$$

If we compare eqs. (6.7) and (6.9) with the corresponding equations (4.8) and (4.17) we see that now supplementary terms arising from the summation over g appear. The inclusion of these terms due to Umklapprozesse has important consequences as may be shown by examining again the conservation laws. The conservation laws of the total number of particles and the total energy remain essentially the same while the conservation of total momentum breaks down. In a system described by the Hamiltonian (6.1), $\mathscr{P}$ is no longer a conserved quantity. One has instead:

$$[\mathscr{P},\, \mathscr{H}^u] = \sum_{q,\, k,\, g} \boldsymbol{g}\, a^\dagger_{k+q+g}\, a_k(b_q + b^\dagger_{-q}). \quad (6.10)$$

From (2.6) and (3.2) it follows that the change of the total momentum due to the electric field is given by

$$\Delta\langle\mathscr{P}\rangle = \frac{-2\pi\, \boldsymbol{E}e}{\omega + i\varepsilon}\left[\frac{1}{2\pi}\langle[\mathscr{P},\, \mathscr{D}]\rangle + \langle\!\langle[\mathscr{P},\, \mathscr{H}^u];\, \mathscr{D}\rangle\!\rangle_{\omega+is}\right] = \frac{-2\pi \boldsymbol{E}e}{\omega + i\varepsilon}\cdot$$

$$\cdot\left\{-\frac{iNI}{2\pi} + \sum_g \boldsymbol{g}[\langle\!\langle a^\dagger_{k+q+g} a_k b_q;\, \mathscr{D}\rangle\!\rangle_{\omega+i\varepsilon} + \langle\!\langle a^\dagger_{k+g+q} a_k b^\dagger_{-q};\, \mathscr{D}\rangle\!\rangle_{\omega+i\varepsilon}]\right\}. \quad (6.11)$$

Replacing the Green's functions on the right hand side of (6.11) by their decoupled expressions which follow directly from (6.5) and (6.6) ,we obtain

$$\Delta\langle\mathscr{P}\rangle = \frac{-2\pi\, \boldsymbol{E}e}{\omega + i\varepsilon}\left\{-\frac{\mathrm{i}NI}{2\pi} + \sum_{k,\, g,\, q} \boldsymbol{g}[(W^{(1)}_{k+q+g,\, k}(\omega+i\varepsilon) + W^{(2)}_{k+q+g,\, k}(\omega+i\varepsilon))\cdot\right.$$

$$\left.\cdot \boldsymbol{G}_{k+q+g}(\omega + i\varepsilon) + W^{(3)}_{k+q+g,\, k}(\omega + i\varepsilon)\, \boldsymbol{D}_q(\omega + i\varepsilon)]\right\}. \quad (6.12)$$

Expressing $\Delta\langle\mathscr{P}\rangle$ with the aid of (2.6) and (5.3) directly in terms of $\boldsymbol{G}_k$ and $\boldsymbol{D}_q$, the following relation for $\boldsymbol{G}_k$ and $\boldsymbol{D}_q$ is obtained:

$$(\omega+i\varepsilon)\,[\sum_k \boldsymbol{k}\, \boldsymbol{G}_k(\omega+i\varepsilon) + \sum_q \boldsymbol{q}\, \boldsymbol{D}_q(\omega+i\varepsilon)] =$$

$$= \left\{-\frac{iNI}{2\pi} + \sum_{k,\, q,\, g} \boldsymbol{g}[(W^{(1)}_{k+q+g,\, k}(\omega+i\varepsilon) + W^{(2)}_{k+q+g,\, k}(\omega+i\varepsilon))\boldsymbol{G}_{k+q+g}(\omega+i\varepsilon) +\right.$$

$$\left. + W^{(3)}_{k+q+g,\, k}(\omega+i\varepsilon)\, \boldsymbol{D}_q(\omega+i\varepsilon)]\right\}. \quad (6.13)$$

Of course this relation which replaces the second equation of (5.6) could

have been derived also from (6.7) and (6.9). For $\omega = 0$ it reduces to

$$\sum_{k,\,g,\,q} \boldsymbol{g}_{\mathrm{L}}^{\mathrm{T}}(W^{(1)}_{k+q-g,\,k}(i\varepsilon) + W^{(2)}_{k+q-g,\,k}(i\varepsilon))\, \boldsymbol{G}_{k+q+g}(i\varepsilon) + \\ + W^{(3)}_{k+q+g,\,k}(i\varepsilon)\, \boldsymbol{D}_q(i\varepsilon)] = \frac{iNI}{2\pi}. \qquad (6.14)$$

which expresses for a static electric field the momentum balance between the momentum put into the system by the electric field per unit time (the right hand side of (6.14)) and the momentum absorbed by the lattice per unit time (the left hand side of (6.14)). Comparing the second relation (5.6) and (6.13), we see that for $\omega = 0$ it is not possible to satisfy (5.6) whereas this is possible for (6.13) or (6.14).

7. *Concluding remarks.* I) Starting from an expression for linear response coefficients given by Kubo's theory and using the many body Green's function methods, a simple systematic derivation for the lowest order contribution (in the electron-phonon coupling) to the frequency dependent complex electrical conductivity tensor $\sigma_{\mu\nu}(\omega)$ is given. As a result a coupled set of linear kinetic equations for the electron and the phonon distribution is obtained. In the particular case of a static field these two equations reduce to linearized Boltzmann equations as can be verified by using the Boltzmann equations given by Peierls[8]). One sees that the change of the phonon distribution (phonon drag) induced by the change of the electron distribution is also a lowest order effect. It follows from our equations that not only in the case of Fermi – Dirac statistics (metals), but also in the limit of low electron density (semiconductors), the phonon drag terms are present in lowest order. Thus also in the case of Boltzmann statistics for the electrons, the assumption of Zubarev[7]) and Fujita[3]) that the phonons remain in thermodynamic equilibrium, is not justified.

II) If the phonon drag is treated properly, one necessarily has to consider the effect of the so called "Umklapprozesse", otherwise the static electrical conductivity becomes infinite. This follows from the fact that without "Umklapprozesse", the total momentum of the electron-phonon system is conserved in the absence of an external field. This total momentum would increase unlimited due to the presence of a static external electric field, unless this increase of momentum is destroyed by "Umklapprozesse". It results also from the coupled set of equations that in this case both the phonon and the electron momentum will become infinite. If one takes into account Umklapprozesse, supplementary terms occur in the kinetic equations for the electron and the phonon distribution. These terms allow the existence of a finite electron and phonon momentum for $\omega = 0$.

III) The derivation here presented does not involve explicitly random phase assumptions or asymptotic conditions (of the type $\lambda \to 0$, $t \to \infty$;

$\lambda^2 t$ remains finite). That only the lowest order terms in the coupling λ_q are obtained is a consequence of the fact that we did already break off in an early stage the chain of equations for Green's functions. It is by no means a restriction of the method. By developing the chain of equations further and decoupling Green's functions of higher order than we considered in this chapter also higher order terms of the conductivity could be obtained. The extension of the derivation to higher order is the subject of the following chapter.

REFERENCES

1) Kubo, R., J. Phys Soc. Japan **12** (1957) 570.
2) Verboven, E., Physica **26** (1961) 1091.
3) Fujita, S. and Abe, R., J. math. Phys. **3** (1962) 350.
   Fujita, S., J. math. Phys. **3** (1962) 1246.
4) Lang, I. G., Sov. Phys. sol. State **2** (1961) 2077.
5) Kohn, W. and Luttinger, J. M., Phys. Rev. **108** (1957) 590.
6) Bonch-Bruevich, V. L. and Tyablikov, S. V., The Green Function method in Statist. Mechanics, Northholland (1962) pag. 104.
7) Zubarev, D. N., Sov. Phys. Uspekhi **3** (1960) 320.
8) Peierls, R E., Quantum Theory of Solids, Oxford (1955) pag. 127.
9) Wilson, A. H., The Theory of Metals, Cambridge (1964) pag. 259

CHAPTER III

HIGHER ORDER TRANSPORT EQUATIONS FOR ELECTRONS AND PHONONS DERIVED FROM THE KUBO FORMULA

Synopsis

Starting from the Kubo expression for the frequency dependent electrical conductivity $\sigma(\omega)$, a set of two coupled transport equations is derived for electrons and phonons The method is based on an extension of Green's function techniques which were used in the previous chapter Using the equations of motion method, the hierarchy of equations for Green's functions is set up to the fourth order By applying decoupling techniques in a systematic way, a closed system of two linear transport equations is obtained In higher order in the electron-phonon coupling, corrections to the collision term as well as to the streaming term of the usual Boltzmann equation are obtained Contrary to the case of electron-impurity scattering, correlation effects which are a direct consequence of the many body character of the system, appear, they affect both the streaming and the collision part of higher order transport equations

1. *Introduction.* In the previous chapter[1]) (hereafter to be referred to as I), the Kubo expression for the frequency dependent electrical conductivity $\sigma(\omega)$ of a system of electrons interacting with lattice phonons was studied by many body Green's function theory[2]). Starting from an electron-hole Green's function, a hierarchy of coupled equations for Green's functions was derived, where lower order Green's functions are expressed in terms of higher order ones The lower members of this in fact infinite hierarchy were truncated by the so-called decoupling technique, a method applied in classical statistics by Bogoljubov[3]). In this way, a closed system of two coupled linear integral equations for both the deviation from equilibrium of the electron distribution and the deviation from equilibrium of the phonon distribution (phonon drag), was obtained. In the case of a static external field ($\omega = 0$), this set of equations reduced to two linearized Boltzmann equations. Due to the fact that the hierarchy was decoupled in an early stage, we obtained only a lowest order result with respect to the electron-phonon coupling λ_q.

In the present chapter we consider further members of the hierarchy which contain higher order Green's functions. By applying decoupling techniques

in a well defined way, it is possible to perform a systematic perturbation development in powers of the electron-phonon coupling. This will be illustrated by the derivation of a set of two transport equations including terms of fourth order in λ_q. Such a development corresponds to a calculation of the static electrical conductivity tensor up to order λ_q^0. The explicit results which we obtain give already more insight in the formal structure of transport equations extended to general order. In particular, a class of terms is found which may be considered as corrections to the streaming term (proportional to the first power of the electrical field) of the usual Boltzmann equation. These terms arise from the combined effect of streaming and collision and correspond to the "interference terms", derived by Kohn and Luttinger in the case of electron-impurity scattering[4]). Among the fourth order corrections to the collision term, one may distinguish between two classes of corrections. A first class are those corrections one would expect from quantum theory including a.o. the renormalization of the electron energy and a shift of the phonon frequency; the second class is given by corrections including correlation effects due to the many body problem character of the electron-phonon system. In the case of elastic scattering of electrons by static impurities, the situation is different. Transport phenomena for such a system have been studied by Kohn and Luttinger[4]) and by Verboven[5]). As shown by the latter author, the Kubo formula then reduces to a one electron formula and no open hierarchy is obtained.

In order to make the present chapter self-contained, we start in section 2. with recalling briefly several basic relations already given in I. In section 3., the hierarchy is constructed by deriving equations of motion for Green's functions of increasing order. Here terms which were neglected in I, are taken into account. The next section is devoted to the explicit evaluation of these correction terms up to terms of order λ_q^0. In section 5., expressions of higher order transport equations for both electrons and phonons are written down and discussed. General considerations on the derivation of a set of two coupled transport equations by including terms of arbitrary high order, are made. Section 6. contains the concluding remarks and a summary of results. The present method is compared with other techniques and results; in particular, a comparison with transport equations derived for the case of electron-impurity scattering, is made. In an appendix, the basic equations for this situation are written down by means of the Green's functions formalism.

2. *Basic Relations.* As a starting point, we recall briefly some definitions and expressions used in I. The Hamiltonian of the system to be considered is given by

$$\mathscr{H} = \sum_k E_k a_k^\dagger a_k + \sum_q \omega_q b_q^\dagger b_q + \sum_{k,q} \lambda_q a_{k+q}^\dagger a_k (b_q + b_{-q}^\dagger). \qquad (2.1)$$

Here $a_k^\dagger$, a_k are the creation and annihilation operators for an electron in the state $|k\rangle$, E_k is the free electron energy while $b_q^\dagger$, b_q and ω_q are the corresponding quantities for phonons ($\hbar = 1$). The factor λ_q determines the coupling between the electron and the phonon field and has the property

$$\lambda_q = \lambda_{-q}. \tag{2.2}$$

In formula (2.1), the $\boldsymbol{k}$-sum runs over thewhole momentum space while the $\boldsymbol{q}$-sum is restricted to the first Brillouin zone. As shown in I, sect. 6, the inclusion of Umklapprozesse offers no additional difficulty. We shall therefore not insist on this point. The external perturbation is given by an electric field $\boldsymbol{E}\exp[-i\omega t + \varepsilon t]$ of frequency ω and the corresponding perturbation Hamiltonian has the form

$$\Delta\mathscr{H} = -\boldsymbol{E}\cdot e\mathscr{D}\exp[-i\omega t + \varepsilon t]. \tag{2.3}$$

In (2.3), $e\mathscr{D}$ is the total dipole moment of the system, e being the electron charge. According to I, eq. (2.14), the electrical conductivity tensor may be written as

$$\sigma_{\mu\nu}(\omega) = \frac{-2\pi e}{V}\sum_k (j_k)_\mu \langle\langle a_k^\dagger a_k;\, \mathscr{D}_\nu\rangle\rangle_{\omega+i\varepsilon}. \tag{2.4}$$

Here V is the total volume of the system, $(j_k)_\mu$ is the μ-th component of the one electron current and $\langle\langle a_k^\dagger a_k;\, \mathscr{D}_\nu\rangle\rangle_{\omega+i\varepsilon}$ is the Fourier transform of the Green's function (see I, eq. (2.2)–(2.6))

$$\langle\langle a_k^\dagger a_k;\, \mathscr{D}_\nu\rangle\rangle_t = -i\theta(t)\langle[a_k^\dagger(t)\, a_k(t),\, \mathscr{D}_\nu(0)]_-\rangle. \tag{2.5}$$

The operators $a_k^\dagger(t)$ and $a_k(t)$ are written in the Heisenberg representation with respect to the Hamiltonian (1.1). They satisfy the following relations to be used frequently hereafter:

$$[a_k^\dagger,\, \mathscr{H}] = -E_k a_k^\dagger - \sum_q \lambda_q a_{k+q}^\dagger (b_q + b_{-q}^\dagger) \tag{2.6}$$

$$[a_k,\, \mathscr{H}] = +E_k a_k + \sum_q \lambda_q a_{k-q}(b_q + b_{-q}^\dagger). \tag{2.7}$$

Similar relations hold for the phonon operators b_q, $b_q^\dagger$:

$$[b_q,\, \mathscr{H}] = \omega_q b_q + \sum_k \lambda_q a_{k-q}^\dagger a_k \tag{2.8}$$

$$[b_q^\dagger,\, \mathscr{H}] = -\omega_q b_q^\dagger - \sum_k \lambda_q a_{k+q}^\dagger a_k. \tag{2.9}$$

As follows from I, the problem consists in the evaluation of the functions

$$\boldsymbol{G}_k(\omega + i\varepsilon) = \langle\langle a_k^\dagger a_k;\, \mathscr{D}_\nu\rangle\rangle_{\omega+i\varepsilon} \tag{2.10}$$

and

$$\boldsymbol{D}_q(\omega + i\varepsilon) = \langle\langle b_q^\dagger b_q;\, \mathscr{D}_\nu\rangle\rangle_{\omega+i\varepsilon}. \tag{2.11}$$

$\boldsymbol{G}_k$ is the deviation from equilibrium of the electron distribution due to the applied external electric field while $\boldsymbol{D}_q$ is the deviation from equilibrium of the phonon distribution, induced by the interaction of the phonons with the driven electrons:

$$\Delta\langle a_k^\dagger a_k\rangle = -2\pi E_\nu \cdot \langle\langle a_k^\dagger a_k;\, \mathscr{D}_\nu\rangle\rangle_{\omega+i\varepsilon} \tag{2.12}$$

$$\Delta\langle b_q^\dagger b_q\rangle = -2\pi E_\nu \cdot \langle\langle b_q^\dagger b_q;\, \mathscr{D}_\nu\rangle\rangle_{\omega+i\varepsilon}. \tag{2.13}$$

3. *The hierarchy of Green's functions.* Generally (see I), the equation of motion for a Green's function $\langle\langle \mathscr{C}_1;\, \mathscr{C}_2\rangle\rangle_{\omega+i\varepsilon}$ where $\mathscr{C}_1$ and $\mathscr{C}_2$ are any operators, is given by

$$(\omega + i\varepsilon)\langle\langle \mathscr{C}_1;\, \mathscr{C}_2\rangle\rangle_{\omega+i\varepsilon} = \frac{1}{2\pi}\langle[\mathscr{C}_1, \mathscr{C}_2]\rangle + \langle\langle[\mathscr{C}_1, \mathscr{H}];\, \mathscr{C}_2\rangle\rangle_{\omega+i\varepsilon}. \tag{3.1}$$

In the following, $\mathscr{C}_2 \equiv \mathscr{D}_\nu$, while $\mathscr{C}_1$ will be a product of electron and phonon annihilation and creation operators. In particular, the equations of motion for the simplest Green's functions (1.10) and (1.11) read

$$z\langle\langle a_k^\dagger a_k;\, \mathscr{D}_\nu\rangle\rangle_z = \frac{1}{2\pi}\langle[a_k^\dagger a_k,\, \mathscr{D}_\nu]\rangle + \sum_q \lambda_q[\langle\langle a_k^\dagger a_{k-q} b_q;\, \mathscr{D}_\nu\rangle\rangle_z +$$

$$+ \langle\langle a_k^\dagger a_{k-q} b_{-q}^\dagger;\, \mathscr{D}_\nu\rangle\rangle_z - \langle\langle a_{k+q}^\dagger a_k b_q;\, \mathscr{D}_\nu\rangle\rangle_z - \langle\langle a_{k+q}^\dagger a_k b_{-q}^\dagger;\, \mathscr{D}_\nu\rangle\rangle_z], \tag{3.2}$$

and

$$z\langle\langle b_q^\dagger b_q;\, \mathscr{D}_\nu\rangle\rangle_z = 0 - \sum_k \lambda_q[\langle\langle a_{k+q}^\dagger a_k b_q;\, \mathscr{D}_\nu\rangle\rangle_z - \langle\langle b_q^\dagger a_{k-q}^\dagger a_k;\, \mathscr{D}_\nu\rangle\rangle_z] \tag{3.3}$$

where use has been made of eqs. (2.6) and (2.7) and $z = \omega + i\varepsilon$. The higher order Green's functions on the right hand side (r.h.s.) of eqs. (3.2), (3.3) satisfy in turn similar equations of motion as for instance (see I, (3.10), (3.11)):

$$(z + E_{k+q} - E_k - \omega_q)\langle\langle a_{k+q}^\dagger a_k b_q;\, \mathscr{D}_\nu\rangle\rangle_z = \frac{1}{2\pi}\langle[a_{k+q}^\dagger a_k b_q,\, \mathscr{D}_\nu]\rangle +$$

$$+ \sum_{q_1} \lambda_{q_1}[\langle\langle a_{k+q}^\dagger a_{k-q_1} b_{q_1} b_q;\, \mathscr{D}_\nu\rangle\rangle_z + \langle\langle a_{k+q}^\dagger a_{k-q_1} b_{-q_1}^\dagger b_q;\, \mathscr{D}_\nu\rangle\rangle_z -$$

$$- \langle\langle a_{k+q+q_1}^\dagger a_k b_{q_1} b_q;\, \mathscr{D}_\nu\rangle\rangle_z - \langle\langle a_{k+q+q_1}^\dagger a_k b_{-q_1}^\dagger b_q;\, \mathscr{D}_\nu\rangle\rangle_z] +$$

$$+ \sum_{k_1} \lambda_q \langle\langle a_{k+q}^\dagger a_k a_{k_1-q}^\dagger a_{k_1};\, \mathscr{D}_\nu\rangle\rangle_z. \tag{3.4}$$

$$(z + E_{k+q} - E_k + \omega_q)\langle\langle a_{k+q}^\dagger a_k b_{-q}^\dagger;\, \mathscr{D}_\nu\rangle\rangle_z = \frac{1}{2\pi}\langle[a_{k+q}^\dagger a_k b_{-q}^\dagger,\, \mathscr{D}_\nu]\rangle +$$

$$+ \sum_{q_1} \lambda_{q_1}[\langle\langle a_{k+q}^\dagger a_{k-q_1} b_{q_1} b_{-q}^\dagger;\, \mathscr{D}_\nu\rangle\rangle_z + \langle\langle a_{k-q}^\dagger a_{k-q_1} b_{q_1}^\dagger b_{-q}^\dagger;\, \mathscr{D}_\nu\rangle\rangle_z -$$

$$- \langle\langle a_{k+q+q_1}^\dagger a_k b_{q_1} b_{-q}^\dagger;\, \mathscr{D}_\nu\rangle\rangle_z - \langle\langle a_{k+q+q_1}^\dagger a_k b_{-q_1}^\dagger b_{-q}^\dagger;\, \mathscr{D}_\nu\rangle\rangle_z] -$$

$$- \sum_{k_1} \lambda_q \langle\langle a_{k+q}^\dagger a_{k_1-q} a_{k_1};\, \mathscr{D}_\nu\rangle\rangle_z. \tag{3.5}$$

The corresponding equations for $\langle\langle a_k^\dagger a_{k-q} b_q ; \mathscr{D}_\nu \rangle\rangle_z$, $\langle\langle a_k^\dagger a_{k-q} b_{-q}^\dagger ; \mathscr{D}_\nu \rangle\rangle_z$ and $\langle\langle a_{k-q}^\dagger a_k b_q^\dagger ; \mathscr{D}_\nu \rangle\rangle_z$ are obtained directly from (3.4) and (3.5) by a change of indices. From equations (3.4) and (3.5) we see that the Green's functions on the left hand side are again expressed by means of even higher order Green's functions on the r.h.s.. For these latter we may in turn construct equations of motion and by continuing further this procedure, we obtain an open chain of coupled equations for Green's functions of increasing order. In the preceeding paper I, the hierarchy was truncated by decoupling the Green's functions on the r.h.s. of (3.4) and (3.5). As remarked in I, $\langle\langle a_k^\dagger a_k ; \mathscr{D}_\nu \rangle\rangle_z$ is the linear correction (due to the electric field) to the equilibrium value of the electron density $\langle a_k^\dagger a_k \rangle = n_k$. Similarly, the Green's function $\langle\langle a_{k+q_1}^\dagger a_{k-q} b_{-q_1}^\dagger b_q ; \mathscr{D}_\nu \rangle\rangle_z$ is the correction to the equilibrium value of the more complicated distribution function $\langle a_{k+q+q_1}^\dagger a_k b_{-q_1}^\dagger b_q \rangle$. By pairing off in all possible ways creation and annihilation operators, this higher order distribution function may be written as

$$\langle a_{k+q+q_1}^\dagger a_k b_{-q_1}^\dagger b_q \rangle = \delta_{q+q_1} \langle b_{-q_1}^\dagger b_q \rangle \langle a_{k+q+q_1}^\dagger a_k \rangle + \text{correction terms}, \quad (3.6)$$

where the correction terms are of higher order in the electron-phonon coupling. δ_x denotes the Kronecker delta: $\delta_x = 1$ for $x = 0$ and zero otherwise. Now perturbing (3.6) by an electric field $\boldsymbol{E} \exp[-i(\omega + i\varepsilon)\, t]$, we obtain in lowest order in $\boldsymbol{E}$ for the deviation caused by $\boldsymbol{E}$:

$$\langle\langle a_{k+q+q_1}^\dagger a_k b_{-q_1}^\dagger b_q ; \mathscr{D}_\nu \rangle\rangle_z = \delta_{q+q_1} \{ v_q \langle\langle a_k^\dagger a_k ; \mathscr{D}_\nu \rangle\rangle_z + n_k \langle\langle b_q^\dagger b_q ; \mathscr{D}_\nu \rangle\rangle_z \} + \\ + \text{correction terms } d_1(z)_{k+q+q_1, k, q}, \quad (3.7)$$

where n_k, v_q are the equilibrium distributions respectively for electrons and phonons. Similarly

$$\langle\langle a_{k+q+q_1}^\dagger a_k b_{q_1} b_{-q}^\dagger ; \mathscr{D}_\nu \rangle\rangle_z = \delta_{q+q_1} \{ (1+v_q) \langle\langle a_k^\dagger a_k ; \mathscr{D}_\nu \rangle\rangle_z + n_k \langle\langle b_{-q}^\dagger b_{-q} ; \mathscr{D}_\nu \rangle\rangle_z \} + \\ + \text{correction terms } d_2(z)_{k+q+q_1, k, q}. \quad (3.8)$$

From

$$\langle a_{k+q}^\dagger a_k a_{k-q}^\dagger a_{k_1} \rangle = \delta_{k+q-k_1} \langle a_k a_{k_1-q}^\dagger \rangle \langle a_{k+q}^\dagger a_{k_1} \rangle + \text{correction terms} \quad (3.9)$$

follows

$$\langle\langle a_{k+q}^\dagger a_k a_{k_1-q}^\dagger a_{k_1} ; \mathscr{D}_\nu \rangle\rangle_z = \delta_{k+q-k_1} \{ (1 - n_k) \langle\langle a_{k+q}^\dagger a_{k+q} ; \mathscr{D}_\nu \rangle\rangle_z - \\ - n_{k+q} \langle\langle a_k^\dagger a_k ; \mathscr{D}_\nu \rangle\rangle_z \} + \text{correction terms } d_3(z)_{k+q, k, k_1}. \quad (3.10)$$

We remark that the Green's function $\langle\langle a_{k+q}^\dagger a_k a_{k_1-q}^\dagger a_{k_1} ; \mathscr{D}_\nu \rangle\rangle_z$ contains only electron operators; expressions of this type correspond to an indirect electron-electron interaction induced by the phonons. By the change of variables $(\boldsymbol{k} + \boldsymbol{q}) \to \boldsymbol{k}$, $\boldsymbol{k} \to (\boldsymbol{k} - \boldsymbol{q})$, one deduces directly from eqs. (3.7)

and (3.8) the corresponding expressions for $\langle\langle a^\dagger_{k+q} a_{k-q_1} b^\dagger_{-q_1} b_{-q}; \mathscr{D}_\nu\rangle\rangle_z$ and $\langle\langle a^\dagger_{k+q} a_{k-q_1} b_{q_1} b^\dagger_{-q}; \mathscr{D}_\nu\rangle\rangle_z$.

The correction terms d_1, d_2 and d_3 of eqs. (3.7), (3.8) and (3.10) contain more complex electron-phonon and electron-electron correlations and are therefore of higher order in the coupling λ_q.

This may be seen by applying the theorem of Bloch and De Dominicis[6]), an extension of Wicks theorem for temperature dependent perturbation theory (see also on this subject the appendix of the paper of Nishikawa and Barrie[7]). From the same theorem it follows that terms as

$$\langle\langle a^\dagger_{k+q} a_{k-q_1} b^\dagger_{-q_1} b^\dagger_q; \mathscr{D}_\nu\rangle\rangle_z \quad \text{and} \quad \langle\langle a^\dagger_{k+q} a_{k-q_1} b_{q_1} b_q; \mathscr{D}_\nu\rangle\rangle_z$$

in eqs. (3.4) and (3.5) are also of higher order in λ_q. As already shown in the appendix of I, terms like $\langle[a^\dagger_{k+q} a_k b_q, \mathscr{D}_\nu]\rangle$ and $\langle[a^\dagger_k a_{k-q} b^\dagger_{-q}, \mathscr{D}_\nu]\rangle$ give also higher order contributions.

Taking into account these remarks, we may write for eq. (3.4) by using (3.7) and (3.10):

$$\begin{aligned}\langle\langle a^\dagger_{k+q} a_k b_q; \mathscr{D}_\nu\rangle\rangle_z = {} & \left\{\frac{\lambda_q}{z + E_{k+q} - E_k - \omega_q}\right\}\{-(\nu_q + n_{k+q})\, \boldsymbol{G}_k(z) + \\ & + (1 + \nu_q - n_k)\, \boldsymbol{G}_{k+q}(z) + (n_{k+q} - n_k)\, \boldsymbol{D}_q(z)\} + \\ & + \frac{1}{2\pi} \cdot \frac{\langle[a^\dagger_{k+q} a_k b_q, \mathscr{D}_\nu]\rangle}{z + E_{k+q} - E_k - \omega_q} + \boldsymbol{C}(z)_{k+q,\,k,\,q} \end{aligned} \tag{3.11}$$

where $\boldsymbol{C}(z)_{k+q,\,k,\,q}$ is given by

$$\begin{aligned}\boldsymbol{C}(z)_{k+q,\,k,\,q} = {} & \left\{\frac{1}{z + E_{k+q} - E_k - \omega_q}\right\}\{\sum_{q_1} \lambda_{q_1}[d_1(z)_{k+q,\,k-q_1,\,q} - \\ & - d_1(z)_{k+q+q_1,\,k,\,q} + \langle\langle a^\dagger_{k+q} a_{k-q_1} b_{q_1} b_q; \mathscr{D}_\nu\rangle\rangle_z - \\ & - \langle\langle a^\dagger_{k+q+q_1} a_k b_{q_1} b_q; \mathscr{D}_\nu\rangle\rangle_z] + \sum_{k_1} \lambda_q d_3(z)_{k+q,\,k,\,k_1}\}. \end{aligned} \tag{3.12}$$

Similarly, by using eq. (3.8), equation (3.5) may be written as

$$\begin{aligned}\langle\langle a^\dagger_{k+q} a_k b^\dagger_{-q}; \mathscr{D}_\nu\rangle\rangle_z = {} & \left\{\frac{\lambda_q}{z + E_{k+q} - E_k + \omega_q}\right\}\{-(1 + \nu_q - n_{k+q})\, \boldsymbol{G}_k(z) + \\ & + (\nu_q + n_k)\, \boldsymbol{G}_{k+q}(z) + (n_{k+q} - n_k)\, \boldsymbol{D}_{-q}(z)\} + \\ & + \frac{1}{2\pi} \cdot \frac{\langle[a^\dagger_{k+q} a_k b^\dagger_{-q}, \mathscr{D}_\nu]\rangle}{z + E_{k+q} - E_k + \omega_q} + \boldsymbol{C}'(z)_{k+q,\,k,\,q} \end{aligned} \tag{3.13}$$

with

$$\begin{aligned}\boldsymbol{C}'(z)_{k+q,\,k,\,q} = {} & \left\{\frac{1}{z + E_{k+q} - E_k + \omega_q}\right\}\{\sum_{q_1} \lambda_{q_1}[d_2(z)_{k+q,\,k-q_1,\,q} - \\ & - d_2(z)_{k+q+q_1,\,k,\,q} + \langle\langle a^\dagger_{k+q} a_{k-q_1} b^\dagger_{-q_1} b^\dagger_{-q}; \mathscr{D}_\nu\rangle\rangle_z - \\ & - \langle\langle a^\dagger_{k+q+q_1} a_k b^\dagger_{-q_1} b^\dagger_{-q}; \mathscr{D}_\nu\rangle\rangle_z] + \sum_{k_1} \lambda_q d_3(z)_{k+q,\,k,\,k_1}\}. \end{aligned} \tag{3.14}$$

The corresponding expressions for $\langle\langle a_k^\dagger a_{k-q} b_q; \mathscr{D}_\nu\rangle\rangle_z$ and $\langle\langle a_k^\dagger a_{k-q} b_{-q}^\dagger; \mathscr{D}_\nu\rangle\rangle_z$ follow directly from (3.11)–(3.14) by a change of indices $(\boldsymbol{k}+\boldsymbol{q}) \to \boldsymbol{k}$ and $\boldsymbol{k} \to (\boldsymbol{k}-\boldsymbol{q})$.

In I, the two last terms on the r.h.s. of eqs. (3.11) and (3.13) have been neglected because they are of higher order in λ_q. Considering only the expressions between braces on the r.h.s. of these equations, one obtains for $\boldsymbol{G}_k(z)$ a linear integral equation of second order in the electron-phonon coupling. In the case of a static external field, this equation reduces to a linearized version of the usual Boltzmann equation (including phonon drag terms). In this equation the field- or streaming term is given by

$$\langle [a_k^\dagger a_k, \mathscr{D}_\nu]\rangle = i \frac{\partial n_k}{\partial k_\nu}$$

while the collision term is build up from lowest order transition probabilities. A similar equation holds for $\boldsymbol{D}_q(z)$.

At present we want to go further and investigate how transport equations look like if one takes into account higher order corrections.

There are two main groups of corrections to be considered:

1) corrections to the usual collision term; we shall see that these corrections are coming from $\boldsymbol{C}(z)_{k+q,k,q}$, $\boldsymbol{C}'(z)_{k+q,k,q}$, $\boldsymbol{C}(z)_{k,k-q,q}$ and $\boldsymbol{C}'(z)_{k,k-q,q}$

2) corrections to the usual streaming term, which are coming from

$$\frac{\langle [a_{k+q}^\dagger a_k b_{-q}^\dagger, \mathscr{D}_\nu]\rangle}{z + E_{k+q} - E_k + \omega_q}, \quad \frac{\langle [a_{k+q}^\dagger a_k b_q, \mathscr{D}_\nu]\rangle}{z + E_{k+q} - E_k - \omega_q}, \quad \frac{\langle [a_k^\dagger a_{k-q} b_{-q}^\dagger, \mathscr{D}_\nu]\rangle}{z + E_k - E_{k-q} + \omega_q}$$

and

$$\frac{\langle [a_k^\dagger a_{k-q} b_q, \mathscr{D}_\nu]\rangle}{z + E_k - E_{k-q} - \omega_q}.$$

We first construct the equations of motions for the different members of the collision term corrections.

Equations (3.7), (3.8) and (3.10) may be written as

$$d_1(z)_{k+q+q_1,k,q} = \langle\langle a_{k+q+q_1}^\dagger a_k b_{-q_1}^\dagger b_q; \mathscr{D}_\nu\rangle\rangle_z - \delta_{q+q_1}[v_q \boldsymbol{G}_k(z) + n_k \boldsymbol{D}_q(z)], \quad (3.15)$$

$$d_2(z)_{k+q+q_1,k,q} = \langle\langle a_{k+q+q_1}^\dagger a_k b_{q_1} b_{-q}^\dagger; \mathscr{D}_\nu\rangle\rangle_z - \delta_{q+q_1}[(1+v_q)\, \boldsymbol{G}_k(z) + n_k \boldsymbol{D}_{-q}(z)], \quad (3.16)$$

$$d_3(z)_{k+q,k,k_1} = \langle\langle a_{k+q}^\dagger a_k a_{k_1-q}^\dagger a_{k_1}; \mathscr{D}_\nu\rangle\rangle_z - \delta_{k+q-k_1}[(1-n_k)\, \boldsymbol{G}_{k+q}(z) - n_{k+q} \boldsymbol{G}_k(z)]. \quad (3.17)$$

The equation of motion for $d_1(z)_{k+q+q_1,k}$ reads

$$(z + E_{k+q+q_1} - E_k + \omega_{q_1} - \omega_q)\langle\langle a_{k+q+q_1}^\dagger a_k b_{-q_1}^\dagger b_q; \mathscr{D}_\nu\rangle\rangle_z -$$

$$- z\delta_{q+q_1}[v_q \boldsymbol{G}_k(z) + n_k \boldsymbol{D}_q(z)] = \frac{1}{2\pi} \langle [a_{k+q+q_1}^\dagger a_k b_{-q_1}^\dagger b_q, \mathscr{D}_\nu]\rangle -$$

$$- \sum_{q_2} \lambda_{q_2}[\langle\langle a^\dagger_{k+q+q_1+q_2} a_k b_{q_2} b^\dagger_{-q_1} b_q ; \mathscr{D}_\nu\rangle\rangle_z + \langle\langle a^\dagger_{k+q+q_1+q_2} a_k b^\dagger_{-q_2} b^\dagger_{-q_1} b_q ; \mathscr{D}_\nu\rangle\rangle_z -$$

$$- \langle\langle a^\dagger_{k+q+q_1} a_{k-q_2} b_{q_2} b^\dagger_{-q_1} b_q ; \mathscr{D}_\nu\rangle\rangle_z - \langle\langle a^\dagger_{k+q+q_1} a_{k-q_2} b^\dagger_{-q_2} b^\dagger_{-q_1} b_q ; \mathscr{D}_\nu\rangle\rangle_z] -$$

$$\sum_{k_1} \lambda_{q_1} \langle\langle a^\dagger_{k+q+q_1} a_k a^\dagger_{k_1-q_1} a_{k_1} b_q ; \mathscr{D}_\nu\rangle\rangle_z + \sum_{k_1} \lambda_q \langle\langle a^\dagger_{k+q+q_1} a_k b^\dagger_{-q_1} a^\dagger_{k_1-q} a_{k_1} ; \mathscr{D}_\nu\rangle\rangle_z -$$

$$-\nu_q \delta_{q+q_1} \left\{ \frac{1}{2\pi} \langle [a^\dagger_k a_k, \mathscr{D}_\nu]\rangle - \sum_{q_2} \lambda_{q_2}[\langle\langle a^\dagger_{k+q_2} a_k b_{q_2} ; \mathscr{D}_\nu\rangle\rangle_z + \right.$$

$$\left. + \langle\langle a^\dagger_{k+q_2} a_k b^\dagger_{-q_2} ; \mathscr{D}_\nu\rangle\rangle_z - \langle\langle a^\dagger_k a_{k-q_2} b_{q_2} ; \mathscr{D}_\nu\rangle\rangle_z - \langle\langle a^\dagger_k a_{k-q_2} b^\dagger_{-q_2} ; \mathscr{D}_\nu\rangle\rangle_z \right\} -$$

$$- n_k \delta_{q+q_1} \sum_{k_1} \lambda_q \{ - \langle\langle a^\dagger_{k_1+q} a_{k_1} b_q ; \mathscr{D}_\nu\rangle\rangle_z + \langle\langle a^\dagger_{k_1-q} a_{k_1} b^\dagger_q ; \mathscr{D}_\nu\rangle\rangle_z \}. \qquad (3.18)$$

Similar equations hold also for $d_2(z)_{k+q-q_1,k}$, $d_3(z)_{k+q,k,k_1}$ and the Green's functions $\langle\langle a^\dagger_{k+q+q_1} a_k b_{q_1} b_q ; \mathscr{D}_\nu\rangle\rangle_z$ and $\langle\langle a^\dagger_{k+q+q_1} a_k b^\dagger_{-q_1} b^\dagger_{-q} ; \mathscr{D}_\nu\rangle\rangle_z$ in the r.h.s. members of equations (3.12) and (3.14). The explicit expressions of these equations are quoted in appendix A.

The terms on the r.h.s. of eqs. (3.18)–(A. 4) may be evaluated by decoupling techniques. This will be done in the next section.

4. *The explicit evaluation of higher order corrections.* At present we want to replace all terms on the r.h.s. of eqs. (3.18)–(A. 4) by their lowest order contributions; this shall be done by using decoupling techniques. The first term on the r.h.s. of (3.18) may be written as

$$\langle [a^\dagger_{k+q+q_1} a_k b^\dagger_{-q_1} b_q, \mathscr{D}_\nu]\rangle = \delta_{q+q_1,\nu_q} \langle [a^\dagger_k a_k, \mathscr{D}_\nu]\rangle + \mathcal{O}(\lambda_q) \qquad (4.1)$$

where $\mathcal{O}(\lambda_q)$ is of higher order in the electron-phonon coupling λ_q. The higher order Green's function on the r.h.s. of eqs. (3.18)–(A. 4) are evaluated by decoupling techniques. The Green's function $\langle\langle a^\dagger_{k+q+q_1+q_2} a_k b_{q_2} b^\dagger_{-q_1} b_q ; \mathscr{D}_\nu\rangle\rangle_z$ on the r.h.s. of (3.18) may be considered as the change due to the external field of the distribution function $\langle a^\dagger_{k+q+q_1+q_2} a_k b_{q_2} b^\dagger_{-q_1} b_q\rangle$. This distribution function may be factorized (decoupled) in terms of simpler correlation functions by pairing off creation and annihilation operators in all possible ways:

$$\langle a^\dagger_{k+q+q_1+q_2} a_k b_{q_2} b^\dagger_{-q_1} b_q\rangle = \delta_{q_2+q_1} \langle b_{-q_1} b^\dagger_{-q_1}\rangle \langle a^\dagger_{k+q} a_k b_q\rangle +$$

$$+ \delta_{q+q_1} \langle b^\dagger_q b_q\rangle \langle a^\dagger_{k+q_2} a_k b_{q_2}\rangle + \mathcal{O}(\lambda_q). \qquad (4.2)$$

We remark that the contribution obtained by pairing off $a^\dagger_{k+q+q_1}$ and a_k i.e. $\delta_{q+q_1+q_2} \langle b_{q_2} b^\dagger_{q+q_2} b_q\rangle \langle a^\dagger_k a_k\rangle$ is of higher order in λ_q and therefore included in higher order terms which we shall not consider explicitly here. Perturbing (4.2) by an electric field $\boldsymbol{E} \exp[-i(\omega + i\varepsilon)\, t]$ and retaining only terms linear

in $\boldsymbol{E}$ yields

$$\langle a^{\dagger}_{k+q+q_1+q_2} a_k b_{q_2} b^{\dagger}_{-q_1} b_q ; \mathscr{D}_\nu \rangle\!\rangle_z =$$

$$= \delta_{q_2+q_1} [\langle a^{\dagger}_{k+q} a_k b_{q_2} \rangle \boldsymbol{D}_{-q_1}(z) + (1 + \nu_{q_1}) \langle\!\langle a^{\dagger}_{k+q} a_k b_q ; \mathscr{D}_\nu \rangle\!\rangle_z] +$$

$$+ \delta_{q+q_1} [\langle a^{\dagger}_{k+q_2} a_k b_{q_2} \rangle \boldsymbol{D}_q(z) + \nu_q \langle\!\langle a^{\dagger}_{k+q_2} a_k b_{q_2} ; \mathscr{D}_\nu \rangle\!\rangle_z] + \mathcal{O}(\lambda_q). \tag{4.3}$$

where $\mathcal{O}(\lambda_q)$ is of higher order in λ_q and shall be neglected in the following. By writing down (4.3) we did made use of the relation $\langle\!\langle b_q b^{\dagger}_q ; \mathscr{D}_\nu \rangle\!\rangle_z = \langle\!\langle b^{\dagger}_q b_q ; \mathscr{D}_\nu \rangle\!\rangle_z \equiv \boldsymbol{D}_q(z)$ which is a direct consequence of the commutation rules for Bose operators. In the same way one finds for the other terms on the r.h.s. of (3.18):

$$\langle\!\langle a^{\dagger}_{k+q+q_1+q_2} a_k b^{\dagger}_{-q_2} b^{\dagger}_{-q_1} b_q ; \mathscr{D}_\nu \rangle\!\rangle_z =$$

$$= \delta_{q+q_1} [\langle a^{\dagger}_{k+q_2} a_k b^{\dagger}_{-q_2} \rangle \boldsymbol{D}_q(z) + \nu_q \langle\!\langle a^{\dagger}_{k+q_2} a_k b^{\dagger}_{-q_2} ; \mathscr{D}_\nu \rangle\!\rangle_z] +$$

$$+ \delta_{q_2+q} [\langle a^{\dagger}_{k+q_1} a_k b^{\dagger}_{-q_1} \rangle \boldsymbol{D}_q(z) + \nu_q \langle\!\langle a^{\dagger}_{k+q_1} a_k b^{\dagger}_{-q_1} ; \mathscr{D}_\nu \rangle\!\rangle_z] + \mathcal{O}(\lambda_q). \tag{4.4}$$

$$\langle\!\langle a^{\dagger}_{k+q+q_1} a_{k-q_2} b_{q_2} b^{\dagger}_{-q_1} b_q ; \mathscr{D}_\nu \rangle\!\rangle_z =$$

$$= \delta_{q_1+q} [\langle a^{\dagger}_k a_{k-q_2} b_{q_2} \rangle \boldsymbol{D}_q(z) + \nu_q \langle\!\langle a^{\dagger}_k a_{k-q_2} b_{q_2} ; \mathscr{D}_\nu \rangle\!\rangle_z] +$$

$$+ \delta_{q_2+q_1} [\langle a^{\dagger}_{k+q-q_2} a_{k-q_2} b_q \rangle \boldsymbol{D}_{q_1}(z) + (1 + \nu_{q_1}) \langle\!\langle a^{\dagger}_{k+q-q_2} a_{k-q_2} b_q ; \mathscr{D}_\nu \rangle\!\rangle_z] + \mathcal{O}(\lambda_q). \tag{4.5}$$

$$\langle\!\langle a^{\dagger}_{k+q+q_1} a_{k-q_2} b^{\dagger}_{-q_2} b^{\dagger}_{-q_1} b_q ; \mathscr{D}_\nu \rangle\!\rangle_z =$$

$$= \delta_{q_1+q} [\langle a^{\dagger}_k a_{k-q_2} b^{\dagger}_{-q_2} \rangle \boldsymbol{D}_q(z) + \nu_q \langle\!\langle a^{\dagger}_k a_{k-q_2} b^{\dagger}_{-q_2} ; \mathscr{D}_\nu \rangle\!\rangle_z] +$$

$$+ \delta_{q_2+q} [\langle a^{\dagger}_{k+q_1-q_2} a_{k-q_2} b^{\dagger}_{-q_1} \rangle \boldsymbol{D}_q(z) + \nu_q \langle\!\langle a^{\dagger}_{k+q_1-q_2} a_{k-q_2} b^{\dagger}_{-q_1} ; \mathscr{D}_\nu \rangle\!\rangle_z] + \mathcal{O}(\lambda_q). \tag{4.6}$$

By remarking that $\langle a^{\dagger}_{k+q+q_1} a_k a^{\dagger}_{k_1-q_1} a_{k_1} b_q \rangle$ may be decomposed into

$$\langle a^{\dagger}_{k+q+q_1} a_k a^{\dagger}_{k_1-q_1} a_{k_1} b_q \rangle =$$

$$= \delta_{q+q_1} \langle a^{\dagger}_k a_k \rangle \langle a^{\dagger}_{k_1-q_1} a_{k_1} b_q \rangle + \delta_{k_1-q_1-k} \langle a^{\dagger}_k a_k \rangle \langle a^{\dagger}_{k+q+q_1} a_{k+q_1} b_q \rangle +$$

$$+ \delta_{k+q+q_1-k_1} \langle a^{\dagger}_{k+q+q_1} a_{k+q+q_1} \rangle \langle a_k a^{\dagger}_{k+q} b_q \rangle + \mathcal{O}(\lambda_q), \tag{4.7}$$

we may write

$$\langle\!\langle a^{\dagger}_{k+q+q_1} a_k a^{\dagger}_{k_1-q_1} a_{k_1} b_q ; \mathscr{D}_\nu \rangle\!\rangle_z =$$

$$= \delta_{q+q_1} [n_k \langle\!\langle a^{\dagger}_{k_1-q_1} a_{k_1} b_q ; \mathscr{D}_\nu \rangle\!\rangle_z + \langle a^{\dagger}_{k_1-q_1} a_{k_1} b_q \rangle G_k(z)] +$$

$$+ \delta_{k_1-q_1-k} [(1 - n_k) \langle\!\langle a^{\dagger}_{k+q+q_1} a_{k+q_1} b_q ; \mathscr{D}_\nu \rangle\!\rangle_z - \langle a^{\dagger}_{k+q+q_1} a_{k+q_1} b_q \rangle G_k(z)] +$$

$$+ \delta_{k+q+q_1-k_1} [-n_{k+q+q_1} \langle\!\langle a^{\dagger}_{k+q} a_k b_q ; \mathscr{D}_\nu \rangle\!\rangle - \langle a^{\dagger}_{k+q} a_k b_q \rangle G_{k+q+q_1}(z)] + \mathcal{O}(\lambda_q), \tag{4.8}$$

where we did made use of the relations $\langle\langle a_k a_k^\dagger; \mathscr{D}_\nu\rangle\rangle_z = -\langle\langle a_k^\dagger a_k; \mathscr{D}_\nu\rangle\rangle_z = -\boldsymbol{G}_k(z)$ and $\langle\langle a_{k+q}^\dagger a_k b_q; \mathscr{D}_\nu\rangle\rangle_z = -\langle\langle a_k a_{k+q}^\dagger b_q; \mathscr{D}_\nu\rangle\rangle_z$ which follow directly from the anticommutation rules for fermion operators.

Similarly

$$\langle\langle a_{k+q+q_1}^\dagger a_k a_{k_1-q}^\dagger a_{k_1} b_{-q_1}^\dagger; \mathscr{D}_\nu\rangle\rangle_z = \delta_{q+q_1}[n_k\langle\langle a_{k_1+q_1}^\dagger a_{k_1} b_{-q_1}^\dagger; \mathscr{D}_\nu\rangle\rangle_z +$$

$$+ \langle a_{k_1+q_1}^\dagger a_{k_1} b_{-q_1}^\dagger\rangle \boldsymbol{G}_k(z)] + \delta_{k+q-q_1}[(1-n_k)\langle\langle a_{k+q+q_1}^\dagger a_{k-q} b_{-q_1}^\dagger; \mathscr{D}_\nu\rangle\rangle_z -$$

$$-\langle a_{k+q+q_1}^\dagger a_{k+q} b_{-q_1}^\dagger\rangle \boldsymbol{G}_k(z)] + \delta_{k+q+q_1-k_1}[-n_{k+q+q_1}\langle\langle a_{k+q_1}^\dagger a_k b_{-q_1}^\dagger; \mathscr{D}_\nu\rangle\rangle_z -$$

$$- \langle a_{k+q_1}^\dagger a_k b_{-q_1}^\dagger\rangle \boldsymbol{G}_{k+q+q_1}(z)] + \mathcal{O}(\lambda_q). \tag{4.9}$$

The quantities like $\langle a_{k+q}^\dagger a_k b_q\rangle$, $\langle a_{k+q}^\dagger a_k b_{-q}^\dagger\rangle$ which occur on the r.h.s. of eqs. (4.3)–(4.9) are mixed electron-phonon distributions; they are correlation functions of higher order in the electron-phonon coupling λ_q. These expressions cannot be factorized directly. It is possible to calculate them by making use of the relation

$$\langle[a_{k+q}^\dagger a_k b_q, \mathscr{H}]\rangle = 0, \tag{4.10}$$

which follows from the invariance of the trace under cyclic permutation. By calculating first (4.10) and by decoupling then the four-operators distribution functions thereby obtained, one finds up to first order in λ_q:

$$\langle a_{k+q}^\dagger a_k b_q\rangle = \lambda_q\left(\frac{\nu_q n_k - (1+\nu_q)\, n_{k+q} + n_{k+q} n_k}{E_k - E_{k+q} + \omega_q}\right). \tag{4.11}$$

In the same way, one obtains

$$\langle a_{k+q}^\dagger a_k b_{-q}^\dagger\rangle = \lambda_q\left(\frac{(1+\nu_q)\, n_k - \nu_q n_{k+q} - n_k n_{k+q}}{E_k - E_{k+q} - \omega_q}\right). \tag{4.12}$$

In order to show explicitly the dependence on λ_q, we write

$$\langle a_{k+q}^\dagger a_k b_q\rangle = \lambda_q \langle a_{k+q}^\dagger a_k b_q\rangle_\lambda \tag{4.13}$$

with

$$\langle a_{k+q}^\dagger a_k b_q\rangle_\lambda = \frac{\nu_q n_k - (1+\nu_q)\, n_{k+q} + n_{k+q} n_k}{E_k - E_{k+q} + \omega_q} \tag{4.14}$$

and

$$\langle a_{k+q}^\dagger a_k b_{-q}^\dagger\rangle = \lambda_q \langle a_{k+q}^\dagger a_k b_{-q}^\dagger\rangle_\lambda \tag{4.15}$$

with

$$\langle a_{k+q}^\dagger a_k b_{-q}^\dagger\rangle_\lambda = \frac{(1+\nu_q)\, n_k - \nu_q n_{k+q} - n_k n_{k+q}}{E_k - E_{k+q} - \omega_q} \tag{4.16}$$

The Green's functions of type $\langle\langle a_{k+q}^\dagger a_k b_q; \mathscr{D}_\nu\rangle\rangle_z$ and $\langle\langle a_{k+q}^\dagger a_k b_{-q}^\dagger; \mathscr{D}_\nu\rangle\rangle_z$ which occur on the r.h.s. of eqs. (4.3), (4.4), (4.5), (4.6), (4.8) and (4.9) may be calculated directly by deriving their equations of motion. By decoupling

and by neglecting terms of higher order in λ_q, one obtains (see eqs. (3.11) and (3.13)):

$$\langle\langle a^\dagger_{k+q} a_k b_q ; \mathscr{D}_\nu \rangle\rangle_z \simeq \lambda_q \Gamma_{k+q,\,k,\,q}(z), \tag{4.17}$$

with $\Gamma_{k+q,\,k,\,q}(z)$ given by

$$\Gamma_{k+q,\,k,\,q}(z) = \left\{ \frac{1}{z + E_{k+q} - E_k - \omega_q} \right\} \{ -(\nu_q + n_{k+q})\, G_k(z) + (1 + \nu_q - n_k)\, G_{k+q}(z) + (n_{k+q} - n_k)\, D_q(z) \}, \tag{4.18}$$

and similarly

$$\langle\langle a^\dagger_{k+q} a_k b^\dagger_{-q} ; \mathscr{D}_\nu \rangle\rangle_z = \lambda_q \Gamma'_{k+q,\,k,\,q}(z), \tag{4.19}$$

with $\Gamma'_{k+q,\,k,\,q}(z)$ given by

$$\Gamma'_{k+q,\,k,\,q}(z) = \left\{ \frac{1}{z + E_{k+q} - E_k + \omega_q} \right\} \{ -(1 + \nu_q - n_{k+q})\, G_k(z) + (\nu_q + n_k)\, G_{k+q}(z) + (n_{k+q} - n_k)\, D_{-q}(z) \}. \tag{4.20}$$

By using eqs. (4.3)–(4.20), one finds from eq. (3.18) and (3.15):

$$\begin{aligned} d_1(z)_{k+q+q_1,\,k,\,q} = \lambda_q \lambda_{q_1} & \left\{ \frac{1}{z + E_{k+q+q_1} - E_k + \omega_{q_1} - \omega_q} \right\} \times \\ & \times \{ -w_{q_1,\,k+q+q_1} \Gamma_{k+q,\,k,\,q}(z) + v_{q_1,\,k} \Gamma_{k+q+q_1,\,k+q_1,\,q}(z) + \\ & + w_{q,\,k} \Gamma'_{k+q+q_1,\,k+q,\,q_1}(z) - v_{q,\,k+q+q_1} \Gamma'_{k+q_1,\,k,\,q_1}(z) + \\ & + (\langle a^\dagger_{k+q+q_1} a_{k+q_1} b_q \rangle_\lambda - \langle a^\dagger_{k+q+q_1} a_{k+q} b^\dagger_{-q_1} \rangle)\, G_k(z) + \\ & + (\langle a^\dagger_{k+q} a_k b_q \rangle_\lambda - \langle a^\dagger_{k+q_1} a_k b^\dagger_{-q_1} \rangle_\lambda)\, G_{k+q+q_1}(z) + \\ & + (\langle a^\dagger_{k+q+q_1} a_{k+q_1} b_q \rangle_\lambda - \langle a^\dagger_{k+q} a_k b_q \rangle_\lambda)\, D_{q_1}(z) + \\ & + (\langle a^\dagger_{k+q+q_1} a_{k+q} b^\dagger_{-q_1} \rangle_\lambda - \langle a^\dagger_{k+q_1} a_k b^\dagger_{-q_1} \rangle_\lambda)\, D_q(z) \}, \end{aligned} \tag{4.21}$$

where

$$v_{q,\,k} = \nu_q + n_k ; \quad w_{q,\,k} = 1 + \nu_q - n_k. \tag{4.22}$$

By making the change of variables $q_1 \leftrightarrow q$, one obtains directly from (4.21) the corresponding expression for $d_2(z)_{k+q+q_1,\,k,\,q}$.

The quantities $d_3(z)_{k+q,\,k,\,k_1}$, $\langle\langle a^\dagger_{k-q+q_1} a_k b_{q_1} b_q ; \mathscr{D}_\nu \rangle\rangle_z$ and $\langle\langle a^\dagger_{k+q+q_1} a_k b^\dagger_{-q_1} b^\dagger_{-q} ; \mathscr{D}_\nu \rangle\rangle_z$ are calculated in a similar way, this is quoted in appendix B. Equations (4.21)–(B. 4) give explicit expressions for all terms which occur in the collision term corrections (3.12) and (3.14).

A second class of corrections, which may be seen as corrections to the streaming term, is found from the consideration of the commutators $\langle [a^\dagger_{k+q} a_k b_q, \mathscr{D}_\nu] \rangle$, $\langle [a^\dagger_{k+q} a_k b^\dagger_{-q}, \mathscr{D}_\nu] \rangle$, $\langle [a^\dagger_k a_{k-q} b_q, \mathscr{D}_\nu] \rangle$ and $\langle [a^\dagger_{k-q} a_k b^\dagger_{-q}, \mathscr{D}] \rangle$ on the r.h.s. of equations (3.4), (3.5) or (3.11), (3.13) and in the corresponding equations for $\langle\langle a^\dagger_k a_{k-q} b_q ; \mathscr{D}_\nu \rangle\rangle_z$ and $\langle\langle a^\dagger_k a_{k-q} b^\dagger_{-q} ; \mathscr{D}_\nu \rangle\rangle_z$.

If one notes that

$$\langle[a^\dagger_{k+q}a_k b_q,\ \mathscr{D}_\nu]\rangle = i\frac{\partial}{\partial k_\nu}\langle a^\dagger_{k+q}a_k b_q\rangle = \lambda_q i\frac{\partial}{\partial k_\nu}\langle a^\dagger_{k+q}a_k b_q\rangle_\lambda \tag{4.23}$$

and

$$\langle[a^\dagger_{k+q}a_k b^\dagger_{-q},\ \mathscr{D}_\nu]\rangle = i\frac{\partial}{\partial k_\nu}\langle a^\dagger_{k+q}a_k b^\dagger_{-q}\rangle = \lambda_q i\frac{\partial}{\partial k_\nu}\langle a^\dagger_{k-q}a_k b^\dagger_{-q}\rangle_\lambda, \tag{4.24}$$

one finds from eqs. (3.4) and (3.5), in addition to the usual streaming term

$$\langle[a^\dagger_k a_k,\ \mathscr{D}_\nu]\rangle = i\frac{\partial n_k}{\partial k_\nu} \tag{4.25}$$

in eq. (3.2), a further contributions

$$\boldsymbol{F}^e_{2;k}(z) = \sum_q[\boldsymbol{F}^e_{2;k+q,k}(z) - \boldsymbol{F}^e_{2;k,k-q}(z)] \tag{4.26}$$

where

$$\boldsymbol{F}^e_{2;k+q,k}(z) = \frac{i}{2\pi}\lambda_q^2\Big[\Big(\frac{1}{z + E_k - E_{k+q} - \omega_q}\Big)\frac{\partial}{\partial k_\nu}\langle a^\dagger_k a_{k+q}b_{-q}\rangle_\lambda + \\ + \Big(\frac{1}{z + E_k - E_{k+q} + \omega_q}\Big)\frac{\partial}{\partial k_\nu}\langle a^\dagger_k a_{k+q}b^\dagger_q\rangle_\lambda\Big]. \tag{4.27}$$

which shows that $\boldsymbol{F}^e_{2;k}(z)$ is a correction of second order in λ_q to the usual streaming term.

5. *The generalized transport equations.* Replacing the third order Green's functions on the right hand side of eq. (3.2) by the r.h.s. expressions of eq. (3.11) and (3.13) yields

$$z\boldsymbol{G}_k(z) = i\frac{\partial n_k}{\partial k_\nu} + \boldsymbol{F}^e_{2;k}(z) + \sum_q \lambda_q^2\{\boldsymbol{\Gamma}_{k,k-q,q}(z) + \boldsymbol{\Gamma}'_{k,k-q,q}(z) - \boldsymbol{\Gamma}_{k+q,k,q}(z) - \\ - \boldsymbol{\Gamma}'_{k+q,k,q}(z)\} + \sum_q \lambda_q\{\boldsymbol{C}_{k,k-q,q}(z) + \boldsymbol{C}'_{k,k-q,q}(z) - \boldsymbol{C}_{k+q,k,q}(z) - \\ - \boldsymbol{C}'_{k+q,k,q}(z)\} \tag{5.1}$$

In this equation, the first r.h.s. term plays the role of the usual field term, obtained from (4.25). $\boldsymbol{F}^e_{2;k}(z)$ stands for the second order corrections to the field or streaming term (see eqs. (4.26) and (4.27)), the first expression between braces gives the lowest order (usual) collision term while the second expression between braces gives corrections to the collision term. By replacing the r.h.s. terms of eqs. (3.12) and (3.14) by their explicit expressions (4.21)–(B. 4), one sees that $\boldsymbol{C}_{k+q,k,q}(z)$,$\boldsymbol{C}'_{k+q,k,q}(z)$ etc. are of third order in λ_q and therefore the last sum in eq. (5.1) yields contributions of fourth order in the electron-phonon coupling λ_q. Remembering the explicit expressions of the quantities $\boldsymbol{\Gamma}_{k,k-q,q}(z)$, $\boldsymbol{\Gamma}'_{k,k-q,q}(z)$ etc., we may write in

a condensed form

$$\sum_q \lambda_q^2\{\boldsymbol{\Gamma}_{k,k-q,q}(z) + \boldsymbol{\Gamma}'_{k,k-q,q}(z) - \boldsymbol{\Gamma}_{k+q,k,q}(z) - \boldsymbol{\Gamma}'_{k+q,k,q}(z)\} = \\ = \sum_{k'} K^{ee}_{2;k,k'}(z)\, \boldsymbol{G}_{k'}(z) + \sum_{q'} K^{ep}_{2;k,q'}(z)\, \boldsymbol{D}_{q'}(z), \qquad (5.2)$$

where the kernels $K^{ee}_{2;k,k'}(z) \equiv W^{ee}_{2;k,k'}(z)$ and $K^{ep}_{2;k,q'}(z) \equiv W^{ep}_{2;k,q'}(z)$ are seen to be lowest order transition probabilities (see I) containing a factor λ_q^2. $W^{ee}_{2;k,k'}$ means that the hierarchy of equations which starts with an electron Green's function $\boldsymbol{G}_k$ is truncated after two equation of motion-steps in order to give again an electron Green's function $\boldsymbol{G}_{k'}$, $W^{ep}_{2;k,q'}$, means that starting from an electron Green's function $\boldsymbol{G}_k$, one breaks off the hierarchy after two steps in order to obtain a phonons Green's function $\boldsymbol{D}_{q'}$.

Inspection of equations (4.21)–(B. 4) shows that the fourth order corrections to the collision term in eq. (5.1) may be written as

$$\sum_q \lambda_q\{\boldsymbol{C}_{k,k-q,q}(z) + \boldsymbol{C}'_{k,k-q,q}(z) - \boldsymbol{C}_{k+q,k,q}(z) - \boldsymbol{C}'_{k+q,k,q}(z)\} = \\ = \sum_{k'} K^{ee}_{4;k,k'}(z)\, \boldsymbol{G}_{k'}(z) + \sum_{q'} K^{ep}_{4;k,q'}(z)\boldsymbol{G}_{q'}(z), \qquad (5.3)$$

where the kernels K_4 are quantities of fourth order in the electron-phonon coupling λ_q, all other indices of these functions having the same signification as for K_2. As concerns the structure of K_4, there is an essential difference between K_2 and K_4. From (4.21)–(B. 4) we see that all contributions to $\boldsymbol{C}_{k+q,k,q}(z)$ etc. and therefore to K_4 may be separated into two parts as follows:

$$K^{ee}_{4;k,k'}(z) = W^{ee}_{4;k,k'}(z) + Q^{ee}_{4;k,k'}(z) \qquad (5.4)$$

$$K^{ep}_{4;k,q'}(z) = W^{ep}_{4;k,q'}(z) + Q^{ep}_{4;k,q'}(x). \qquad (5.5)$$

Here the functions $W_4(z)$ are build up from all terms containing products of two of the quantities u, v, w defined by (4.22) and (B. 2).

All terms of the form $x\boldsymbol{\Gamma}$ and $x\boldsymbol{\Gamma}'$ with $x = u$, v or w in expressions (4.21)–(B. 4) contribute therefore to $W^{ee}_{4;k,k'}(z)$ or $W^{ep}_{4;k,q'}(z)$. The quantities $Q_4(z)$ include all terms in eq. (4.21)–(B. 4) which contain correlation functions like $\langle a^\dagger_{k+q} a_k b_q\rangle$, $\langle a^\dagger_{k+q} a_k b^\dagger_{-q}\rangle$ etc.

Let us now examine in more detail the structure of W_4 and Q_4. All terms contributing to W_4 arise from two phonon processes in such a way that one may distinguish between successive single phonon interactions as is shown by the products of pairs of u, v, w. In other words, an higher order interaction is given by a product of squared matrix elements describing emission or absorption of a single phonon or creation and annihilation of an electron-hole pair. These corrections are those one would expect from quantum theory by considering corrections to the Born approximation, vertex function corrections and renormalization of the electron and the phonon energies.

The latter type of corrections may be isolated easily. We first rewrite expression (3.11) by using (4.17):

$$\ll a^{\dagger}_{k+q} a_k b_q ; \mathscr{D}_{\nu} \gg = \lambda_q \Gamma_{k+q,\, k,\, q}(z) + \frac{1}{2\pi} \frac{\langle [a^{\dagger}_{k+q} a_k b_q ,\, \mathscr{D}_{\nu}] \rangle}{z + E_{k+q} - E_k - \omega_q} + C_{k+q,\, k,\, q}(z), \tag{5.7}$$

with $C_{k+q,\, k,\, q}(z)$ given by (3.12) i.e.

$$C_{k+q,\, k,\, q}(z) = \left\{ \frac{1}{z + E_{k+q} - E_k - \omega_q} \right\} \{ \sum_{q_1} \lambda_{q_1} [d_{1k+q,\, k-q_1,\, q}(z) - d_{1k+q+q_1,\, k,\, q}(z) +$$

$$+ \ll a^{\dagger}_{k+q} a_{k-q_1} b_{q_1} b_q ; \mathscr{D}_{\nu} \gg_z - \ll a^{\dagger}_{k+q+q_1} b_{q_1} b_q ; \mathscr{D}_{\nu} \gg_z] + \sum_{k_1} \lambda_q d_{3k+q,\, k,\, k_1}(z) \}. \tag{5.8}$$

where the r.h.s. terms have to be replaced by their explicit expressions (4.21), (B. 1) and (B. 2). In these latters we collect all terms containing as a factor the function $\Gamma_{k+q,\, k,\, q}(z)$ and write down their contributions $R_{k+q,k,q}(i\varepsilon)$ included in $C_{k+q,\, k,\, q}(z)$, for the case of zero frequency ($\omega = 0$, $z = i\varepsilon$). This gives

$$R_{k+q,\, k,\, q}(i\varepsilon) = \left\{ \frac{\lambda_q \Gamma_{k+q,\, k,\, q}(i\varepsilon)}{E_{k+q} - E_k - \omega_q + i\varepsilon} \right\} \Bigg\{ \sum_{q_1} \lambda^2_{q_1} \Bigg[\frac{w_{q_1,\, k+q+q_1}}{E_{k+q+q_1} - E_k - \omega_q + \omega_{q_1} + i\varepsilon} +$$

$$+ \frac{v_{q_1,\, k+q+q_1}}{E_{k+q+q_1} - E_k - \omega_q - \omega_{q_1} + i\varepsilon} \Bigg] +$$

$$+ \sum_{q_1} \lambda^2_{q_1} \Bigg[\frac{w_{q_1,\, k+q_1}}{E_{k+q} - E_{k+q_1} - \omega_q - \omega_{q_1} + i\varepsilon} +$$

$$+ \frac{v_{q_1,\, k+q_1}}{E_{k+q} - E_{k+q_1} - \omega_q + \omega_{q_1} + i\varepsilon} \Bigg] +$$

$$+ \lambda^2_q \sum_{k_1} \frac{u_{k_1-q,\, k_1}}{E_{k+q} - E_k + E_{k_1-q} - E_{k_1} + i\varepsilon} \Bigg\}, \tag{5.9}$$

where

$$\Gamma_{k+q,\, k,\, q}(i\varepsilon) = \frac{1}{E_{k+q} - E_k - \omega_q + i\varepsilon} [-(1 + \nu_q - n_{k+q})\, G_k(i\varepsilon) +$$

$$+ (\nu_q + n_k)\, G_{k+q}(i\varepsilon) + (n_{k+q} - n_k)\, D_q(i\varepsilon)]. \tag{5.10}$$

We put the definitions

$$\Delta E_k \equiv M_k - \frac{i}{2} \gamma_k = \sum_{q_1} \lambda^2_{q_1} \Bigg[\frac{w_{q_1,\, k+q_1}}{E_{k+q} - E_{k+q_1} - \omega_q - \omega_{q_1} + i\varepsilon} +$$

$$+ \frac{v_{q_1,\, k+q_1}}{E_{k+q} - E_{k+q_1} - \omega_q + \omega_{q_1} + i\varepsilon} \Bigg], \tag{5.11}$$

with

$$M_k = \sum_{q_1} \lambda_{q_1}^2 \mathscr{P} \left[\frac{w_{q_1, k+q_1}}{E_{k+q} - E_{k+q_1} - \omega_q - \omega_{q_1}} + \right.$$
$$\left. + \frac{v_{q_1, k+q_1}}{E_{k+q} - E_{k+q_1} - \omega_q + \omega_{q_1}} \right] \quad (5.12)$$

($\mathscr{P}$ denotes the principal part)

and

$$\gamma_k = 2\pi \sum_{q_1} \lambda_{q_1}^2 [w_{q_1, k+q_1} \delta(E_{k+q} - E_{k+q_1} - \omega_q - \omega_{q_1}) +$$
$$+ v_{q_1, k+q_1} \delta(E_{k+q} - E_{k+q_1} - \omega_q + \omega_{q_1})]. \quad (5.13)$$

We also write

$$\Delta E_{k+q}^* \equiv M_{k+q}^* + \frac{i}{2} \gamma_{k+q}^* = \sum_{q_1} \lambda_{q_1}^2 \left[\frac{w_{q_1, k+q+q_1}}{E_k - E_{k+q+q_1} + \omega_q - \omega_{q_1} - i\varepsilon} + \right.$$
$$\left. + \frac{v_{q_1, k+q+q_1}}{E_k - E_{k+q+q_1} + \omega_q + \omega_{q_1} - i\varepsilon} \right], \quad (5.14)$$

with

$$M_{k+q}^* = \sum_{q_1} \lambda_{q_1}^2 \mathscr{P} \left[\frac{w_{q_1, k+q+q_1}}{E_k - E_{k+q+q_1} + \omega_q - \omega_{q_1}} + \right.$$
$$\left. + \frac{v_{q_1, k+q+q_1}}{E_k - E_{k+q+q_1} + \omega_q + \omega_{q_1}} \right] \quad (5.15)$$

and

$$\gamma_{k+q}^* = 2\pi \sum_{q_1} \lambda_{q_1}^2 [w_{q_1, k+q+q_1} \delta(E_k - E_{k+q+q_1} + \omega_q - \omega_{q_1}) +$$
$$+ v_{q_1, k+q+q_1} \delta(E_k - E_{k+q+q_1} + \omega_q + \omega_{q_1})] \quad (5.16)$$

and we finally put

$$\Delta\omega_q \equiv P_q - \frac{i}{2} \gamma_q = \sum_{k_1} \lambda_q^2 \frac{u_{k_1-q, k_1}}{E_{k+q} - E_k + E_{k_1-q} - E_{k_1} + i\varepsilon} \quad (5.17)$$

with

$$P_q = \sum_{k_1} \lambda_q^2 \mathscr{P} \left[\frac{u_{k_1-q, k_1}}{E_{k+q} - E_k + E_{k_1-q} - E_{k_1}} \right] \quad (5.18)$$

and

$$\gamma_q = 2\pi \sum_{k_1} \lambda_q^2 u_{k_1-q, k_1} \delta(E_{k+q} - E_k + E_{k_1-q} - E_{k_1}) \quad (5.19)$$

The quantities M_k and M_{k+q}^* have a simple physical meaning. They represent the energy shift of an electron and a hole sourrounded by the phonon cloud and play the same role as the so-called mass operator in quantum electrodynamics. Similarly, P_q gives the frequency shift for phonons and may be considered as a polarization operator. The functions γ_k, γ_{k+q}^* and

γ_q, which depend also on the temperature have the meaning of damping factors, they give the reciprocal of the lifetime of the considered particle states. The expressions given here for renormalization and damping of electron and phonon correspond with the formulas calculated in papers 2), 8) by means of one particle Green's functions.

With the help of (5.9), (5.11), (5.14) and (5.17) we may write

$$\frac{\lambda_q}{(E_{k+q} + \Delta E^*_{k-q}) - (E_k + \Delta E_k) - (\omega_q + \Delta\omega_q) + i\varepsilon} [-(1 + \nu_q - n_{k+q}) \boldsymbol{G}_k(i\varepsilon) + (\nu_q + n_k) \boldsymbol{G}_{k+q}(i\varepsilon) + (n_{k+q} - n_k) \boldsymbol{D}_q(i\varepsilon)] =$$
$$= \lambda_q \boldsymbol{\Gamma}_{k+q,k}(i\varepsilon) + \boldsymbol{R}_{k+q,k}(i\varepsilon) + \text{higher order terms} \qquad (5.20)$$

This shows that the contributions $\boldsymbol{R}_{k+q,k}(i\varepsilon)$ of $\boldsymbol{C}_{k+q,k}(i\varepsilon)$ may be obtained by replacing the energies in the denominator of the first r.h.s. term in (3.11) by their corrected complex values (5.11), (5.14) and (5.17). Analogous manipulations can be carried out also for the function $\langle\langle a^\dagger_{k+q} a_k b^\dagger_{-q}; \mathscr{D}_\nu \rangle\rangle_z$ given by eq. (3.13).

By taking together the coefficients of $\boldsymbol{G}_k$, $\boldsymbol{G}_{k+q}$ and $\boldsymbol{D}_q$ in the remaining terms of W_4, it is possible to pick out corrections to $v_{q,k+q}$, $w_{q,k}$ and $u_{k+q,k}$. These corrections would play the role of transition probability corrections and are not essentially different from these found in earlier work on electron-impurity scattering[4) 5) 9)]. The main characteristic of all terms belonging to W_4 is that here an higher order interaction is seen to be build up of products of lowest order processes.

This picture no longer holds for the second class of corrections to the collision term. In the contributions to Q_4, an essentially new aspect appears. The occurence of many particle density matrices as for instance $\langle a^\dagger_{k+q} a_k b_q \rangle$ and $\langle a^\dagger_{k+q} a_k b^\dagger_{-q} \rangle$ is a consequence of the many-body problem character of the electron-phonon system we are considering. The mixed electron-phonon density matrices are correlation type functions; as we have seen in the foregoing section eq. (4.11)–(4.12), these quantities are of higher order in the electron-phonon coupling λ_q and proportional to the first power of the electron density n_k. From a physical point of view, one would say, that when the system is fairly dense, the particles never get away from other particles in the system. Such correlation effects are often neglected or at most treated in a more phenomenological way by assuming the existence of an effective field. In doing so one assumes that each particle of a many-body system moves independently of the others, albeit via a force field depending upon some average parameters of the whole system. This picture is rather incomplete and in a more correct theory, correlations between particles have to be taken into account explicitly. In particular this is the case for a quantum mechanical system. In terms of wave functions one would say that a wave function of a single particle is smeared out over a large part

of the system and therefore there is overlap with wave functions of other particles. The particles may no longer be considered as propagating freely in between collisions, quantum mechanically, they are always in interaction. This effect is pointed out also by Kadanoff and Baym[10]).

The correlation between particles manifests itself not only in the Q_4-contributions to the collision term but affects also the streaming term. In addition to the usual field (streaming) term $i(\partial n_k/\partial k)$ we have obtained the corrections $F^e_{2;k}(z)$ given by eqs. (4.26) and (4.27) and which are of second order in λ_q. This fact again shows that the picture of independent particles in between collision breaks down if one goes to higher order in the electron-phonon coupling. Instead of free electrons, one sees that complex particle correlations are driven by the applied external field[11]). The corrections $F^e_{2;k}(z)$ may be seen as arising from the combined effect of streaming and collision. In this respect, they may be compared directly with the "interference terms" given by Kohn and Luttinger[4]), eq. (85) in the case of electron-impurity scattering. This comparison is made in appendix C of the present paper where the basic equations for the electron-impurity system are written down in terms of Green's function formalism. Recently, also Davis and Résibois have investigated the interference between the external field and the interactions between the particles of the system in the case of plasmas and electrolytes[16]).

Another class of corrections to the streaming term is originating in the case of the electron-impurity scattering from corrections to the Fermi-Dirac distribution. Analogous corrections may be found in our treatment if we recall that the statistical average in the expressions

$$\langle [a_k^\dagger a_k, \mathscr{D}_r] \rangle = i \frac{\partial}{\partial k_r} \langle a_k^\dagger a_k \rangle = i \frac{\partial n_k}{\partial k_r} \tag{5.21}$$

is taken with respect to the full Hamiltonian (1.1). The quantity $\langle a_k^\dagger a_k \rangle$ may be calculated by means of one particle Green's functions theory[2]). By including terms up to second order in λ_q, one finds

$$n_k = \langle a_k^\dagger a_k \rangle = \frac{1}{e^{\beta(E+\Delta E_k)} + 1}; \qquad \left(\beta = \frac{1}{k_B T}\right) \tag{5.22}$$

with

$$\Delta E_k = \mathscr{P} \sum_q \lambda_q^2 \left[\frac{1 + \nu_q - n_{k-q}}{E_k - E_{k-q} - \omega_q} + \frac{n_{k-q} + \nu_q}{E_k - E_{k-q} + \omega_q} \right]. \tag{5.23}$$

By making a series development in ΔE_k, (5.21) becomes

$$i \frac{\partial}{\partial k} \langle a_k^\dagger a_k \rangle = i \frac{\partial}{\partial k} \left[\frac{1}{e^{\beta E_k} + 1} + \Delta E_k \frac{\partial}{\partial E} \left(\frac{1}{e^{\beta E} + 1} \right) \Big|_{E=E_k} + \ldots \right] \tag{5.24}$$

where ΔE_k is given by (5.23). This second type of corrections to the streaming

term is due to the renormalization of the electron energy whereas the corrections $F^e_{2;k}(z)$ are due to the interference between streaming and collision. This fact is also responsible for the existence of streaming terms (of higher order in λ_q) in the transport equation for phonons which will be considered at present.

By making use of (3.11) and (3.13), equation (3.3) may be written as

$$zD_q(z) = F^p_{2;q}(z) - \sum_k \lambda_q^2[\Gamma_{k+q,k,q}(z) - \Gamma'_{k-q,k,-q}(z)] - \\ - \sum_k \lambda_q [C_{k+q,k,q}(z) - C'_{k-q,k,-q}(z)], \qquad (5.25)$$

where

$$F^p_{2;q}(z) = -\frac{i}{2\pi}\lambda_q^2 \sum_k \left[\left(\frac{1}{z + E_{k+q} - E_k - \omega_q}\right)\frac{\partial}{\partial k_\nu}\langle a^\dagger_{k+q} a_k b_q\rangle_\lambda - \right. \\ \left. - \left(\frac{1}{z - E_{k-q} - E_k + \omega_q}\right)\frac{\partial}{\partial k_\nu}\langle a^\dagger_{k-q} a_k b^2_q\rangle_\lambda\right] \qquad (5.26)$$

and where $\Gamma'_{k-q,k,-q}(z)$ and $C'_{k-q,k,-q}(z)$ are obtained from the corresponding expressions (4.20) and (3.14) by a change of indices. By taking into account the explicit expressions for Γ and Γ'', we see that we may put

$$-\sum_k \lambda_q^2[\Gamma_{k+q,k,q}(z) - \Gamma'_{k-q,k,-q}(z)] = \sum_{k'} K^{pe}_{2;q,k'}(z) G_{k'}(z) + \\ + \sum_{q'} K^{pp}_{2;q,q'}(z)\, D_{q'}(z). \qquad (5.27)$$

Here the indices of $K^{pe}_{2;q,k'}(z)$ mean that the hierarchy of equations which begins with a phonon Green's function D_q, was broken off after two equation of motion steps yielding an electron Green's function $G_{k'}$, similarly $K^{pp}_{2;q,k'}(z)$, means that starting from D_q, a phonon Green's function $D_{q'}$ was obtained after two equations of motion and subsequent decoupling.

Quite analogously, we may write for the fourth order corrections to the collision term

$$-\sum_k \lambda_q[C_{k+q,k,q}(z) - C'_{k-q,k,-q}(z)] = \sum_{k'} K^{pe}_{4;q,k'}(z) G_{k'}(z) + \\ + \sum_{q'} K^{pp}_{4;q,q'}(z)\, D_{q'}(z). \qquad (5.28)$$

Here the kernels K_4 may again be separated into two parts as follows

$$K^{pe}_{4;q,k'}(z) = W^{pe}_{4;q,k'}(z) + Q^{pe}_{4;q,k'}(z) \qquad (5.29)$$

$$K^{pp}_{4;q,q'}(z) = W^{pp}_{4;q,q'}(z) + Q^{pp}_{4;q,q'}(z) \qquad (5.30)$$

where Q_4 contain all correlation type corrections.

It is well known that in first approximation (zeroth order), there exists no streaming term for the phonon transport equation. If one goes to second

order in λ_q there appears a streaming term $F^p_{2;q}(z)$ due to correlations of the phonons with the electrons.

This again shows that in higher order in the electron-phonon coupling, the independent particle (electron or phonon) picture is no more valid.

From the foregoing one sees that it is in principle possible to extend the derivation of linear transport equations for electrons and phonons to arbitrary high order in the interaction.

In condensed form, these equations would look like

$$z\boldsymbol{G}_k(z) = i\frac{\partial n_k}{\partial k_\nu} + \sum_{2S} \boldsymbol{F}^e_{2S;k}(z) + \sum_{k'2s} K^{ee}_{2S;k,k'2s}(z)\, \boldsymbol{G}_{k'2s}(z) + \sum_{q'2s} K^{ep}_{2S;k,q'2s}(z)\, \boldsymbol{D}_{q'2s}(z) \tag{5.31}$$

$$z\boldsymbol{D}_q(z) = \sum_{2S} \boldsymbol{F}^p_{2S;q}(z) + \sum_{k'2s} K^{pe}_{2S;q,k'2s}(z)\, \boldsymbol{G}_{k'2s}(z) + \sum_{q'2s} K^{pp}_{2S;q,q'2s}(z)\, \boldsymbol{D}_{q'2s}(z) \tag{5.32}$$

with $S = 1, 2, 3 \ldots\ldots$; $2S$ being the order in the electron-phonon coupling.

Equations similars to (5.31) and (5.32) have been written down by Van Leeuwen who used diagram considerations[13]).

In terms of diagrams, the decoupling of Green's functions is equivalent with the extraction of all "dangerous diagrams". Although the two approaches are different, one obtains essentially analogous results. In particular, our streaming term and streaming term corrections $\boldsymbol{F}^e_{2;k}(z)$, $\boldsymbol{F}^p_{2;q}(z)$ correspond to the class of "non dangerous diagrams" $\mathcal{G}^{nd}_k(\omega)$ and $\boldsymbol{D}^{nd}_q(\omega)$ of Van Leeuwen (see expressions (3.3) and (3.6) of 13)).

By writing down explicitly results according to Van Leeuwen's method, one would also obtain correlation type corrections to the collision term.

6. *Conclusions.* 1. As has been pointed out by Nishikawa and Barrie[7]), the theorem of Bloch and de Dominicis[6]) gives a justification for the use of decoupling techniques. In the case of weak electron-phonon interaction, decoupling is equivalent with perturbation theory. By deriving equations of motion for differences between decoupled and undecoupled expressions and by decoupling the result in a later stage, we did perform perturbation theory in a systematic way. In comparison with diagram techniques, it seems that decoupling method is more direct if one wants to obtain explicit results, as for example correlation effects.

2. If we compare the present derivation of quantum transport equations with the generalized Boltzmann equation derived from the truncation of the B-B-G-Y-K hierarchy in classical statistical mechanics[12]) we have to take into account that in the case of our system, the streaming term is due to the action of the applied external field while for the generalized Boltzmann equation in classical statistics, the streaming is due to spatial inhomogeneities in the system and the distribution functions depend on the spatial

coordinate $\boldsymbol{r}$. Nevertheless there exists a certain formal analogy between the classical transport equations derived by Bogoljubov's method and our quantum mechanical transport equations, in particular the streaming term corrections have a quite similar structure and are due in both cases to correlation effects. One also notes in both cases the occurence of correlation effects in the collision terms; in the quantum mechanical case these effects are seen to be directly dependent on the particle density.

3. An important difference exists between the present problem and the derivation of transport equations for the case of scattering by static impurities. In the latter case, the problem may be reduced to a one electron problem, the electron being elastically scattered by the impurities. As is shown in an appendix, one obtains no hierarchy but the Green's function $\langle\langle a_k^\dagger a_k; \mathscr{D}_\nu \rangle\rangle_z$ is expressed in terms of non diagonal Green's functions like $\langle\langle a_k^\dagger a_{k'}; \mathscr{D}_\nu \rangle\rangle_z$. These latter in turn admit equations of motion (see A.5) and give rise to commutators of the form $\langle [a_k^\dagger a_{k'}, \mathscr{D}_\nu] \rangle$, instead of $\langle [a_{k+q}^\dagger a_k b_q, \mathscr{D}_\nu] \rangle$ for the electron-phonon problem. In this respect the "interference terms" of Kohn and Luttinger arising from $\langle [a_k^\dagger a_{k'}, \mathscr{D}_\nu] \rangle$ are comparable to our streaming term corrections arising from $\langle [a_{k+q}^\dagger a_k b_q, \mathscr{D}_\nu] \rangle$.

4. Recently, several authors have derived kinetic equations for the one electron density matrix in the case of electron-electron and electron-phonon scattering[14) 15)]. The method presented in these papers allows a correct calculation of the collision term, including higher order effects in the electron-electron or electron-phonon interaction. In order to evaluate correctly transport coefficients and to obtain also corrections to the streaming term, one would have to deal with a full Hamiltonian $\mathscr{H}_T$ containing a first part $\mathscr{H}_P$ describing the system of interacting particles and a second part $\mathscr{H}_F$ referring to the interaction with the external field. By constructing the hierarchy for density matrices and by applying decoupling techniques, one would obtain transport equations which after linearization (in the external field), should correspond exactly to our transport equations derived from Kubo formalism by using Green's functions theory.

7. *Summary of results.* At present we want to recall briefly what has been achieved in this chapter. Kubo's expression for the frequency dependent electrical conductivity is written down in terms of Fourier transforms of Green's functions $\langle\langle a_k^\dagger a_k; \mathscr{D}_\nu \rangle\rangle_{\omega+i\varepsilon}$ and $\langle\langle b_q^\dagger b_q; \mathscr{D}_\nu \rangle\rangle_{\omega+i\varepsilon}$ respectively for electrons and phonons. By using the equation of motion method, the first two stages of the hierarchy of equations for Green's functions of increasing order are derived. Green's functions of type $\langle\langle a_{k+q+q_1}^\dagger a_{-q}^\dagger b_{q_1}; \mathscr{D}_\nu \rangle\rangle_z$ are decoupled yielding contributions which correspond to the λ_q^2-terms of the usual Boltzmann equations. By taking into account Green's functions of type $\langle\langle a_{k+q+q_1}^\dagger a_k b_{q_1} b_q; \mathscr{D}_\nu \rangle\rangle_z$, $\langle\langle a_k^\dagger a_{k+q+q1} b_{q_1}^\dagger b_q; \mathscr{D}_\nu \rangle\rangle_z$ and by considering the quantities neglected through the decoupling approximation, the hierarchy

is extended up to the fourth stage. Decoupling of the Green's functions of even higher order thereby obtained yields corrections to the collision term of the transport equations. The corrections to the collision term which are of fourth order in the electron-phonon interaction may be divided into two classes. A first class of corrections includes those which are build up from products of squared matrix elements describing single phonon exchange or annihilation of an electron-hole pair. The second class of corrections to the collision terms contains essentially correlation-type functions. These correlation effects are specific to a many problem and occur also in a part of the corrections to the streaming term. These streaming term corrections may be seen as arising from the combined effect of streaming and collision, they are present in both the transport equations for electrons and phonons and they cannot be obtained by the usual Boltzmann equation approach. From the present derivation of transport equations it may be seen how calculations run to arbitrary high order.

APPENDIX A

Here we write down the explicitly some equations and expressions mentioned in section 3.

Applying an equation of motion like (3.1) to each member on the r.h.s. of (3.16), we see that $d_2(z)_{k+q+q_1,\,k,\,q}$ satisfies

$$
\begin{aligned}
&(z + E_{k+q+q_1} - E_k + \omega_q - \omega_{q_1})\langle\langle a^\dagger_{k+q+q_1} a_k b_{q_1} b^\dagger_{-q};\, \mathscr{D}_\nu\rangle\rangle_z - \\
&- z\delta_{q+q_1}[(1 + \nu_q)\, G_k(z) + n_k D_{-q}(z)] = -\frac{1}{2\pi}\langle[a^\dagger_{k+q+q_1} a_k b_{q_1} b^\dagger_{-q};\, \mathscr{D}_\nu]\rangle - \\
&- \sum_{q_2} \lambda_{q_2}[\langle\langle a^\dagger_{k+q+q_1+q_2} a_k b_{q_2} b_{q_1} b^\dagger_{-q};\, \mathscr{D}_\nu\rangle\rangle_z + \langle\langle a^\dagger_{k+q+q_1+q_2} a_k b^\dagger_{-q_2} b_{q_1} b^\dagger_{-q};\, \mathscr{D}_\nu\rangle\rangle_z - \\
&- \langle\langle a^\dagger_{k+q+q_1} a_{k-q_2} b_{q_2} b^\dagger_{-q_1} b_q;\, \mathscr{D}_\nu\rangle\rangle_z - \langle\langle a^\dagger_{k+q+q_1} a_{k-q_2} b^\dagger_{-q_1} b_{q_1} b^\dagger_{-q};\, \mathscr{D}_\nu\rangle\rangle_z] - \\
&+ \sum_{k_1} \lambda_{q_1} \langle\langle a^\dagger_{k+q+q_1} a_k a^\dagger_{k_1-q_1} a_{k_1} b^\dagger_{-q};\, \mathscr{D}_\nu\rangle\rangle_z - \sum_{k_1} \lambda_q \langle\langle a^\dagger_{k+q+q_1} a_k b_{q_1} a^\dagger_{k_1-q} a_{k_1};\, \mathscr{D}_\nu\rangle\rangle_z - \\
&- (1 + \nu_q)\, \delta_{q+q_1}\left\{\frac{1}{2\pi}\langle[a^\dagger_k a_k,\, \mathscr{D}_\nu]\rangle - \sum_{q_2} \lambda_{q_2}[\langle\langle a^\dagger_{k+q_2} a_k b_{q_2};\, \mathscr{D}_\nu\rangle\rangle_z + \right. \\
&\left. + \langle\langle a^\dagger_{k+q_2} a_k b_{-q_2};\, \mathscr{D}_\nu\rangle\rangle_z - \langle\langle a^\dagger_k a_{k-q_2} b_{q_2};\, \mathscr{D}_\nu\rangle\rangle_z - \langle\langle a^\dagger_k a_{k-q_2} b^\dagger_{-q_2};\, \mathscr{D}_\nu\rangle\rangle_z]\right\} - \\
&- n_k \delta_{q+q_1} \sum_{k_1} \lambda_q\{-\langle\langle a^\dagger_{k_1-q} a_{k_1} b_{-q};\, \mathscr{D}_\nu\rangle\rangle_z + \langle\langle a_{k_1+q} a_{k_1} b^\dagger_{-q};\, \mathscr{D}_\nu\rangle\rangle_z\} \qquad \text{(A. 1)}
\end{aligned}
$$

A similar equation holds for $d_3(z)_{k+q+q_1,\,k}$

$$(z + E_{k+q} - E_k + E_{k_1-q} - E_{k_1})\langle\langle a^\dagger_{k+q}a_k a^\dagger_{k_1-q}a_{k_1};\,\mathscr{D}_\nu\rangle\rangle_z -$$

$$- z\delta_{k+q-k_1}[(1 - n_k)\,G_{k+q}(z) - n_{k+q}G_k(z)] =$$

$$= \frac{1}{2\pi}\langle[a^\dagger_{k-q}a_k a^\dagger_{k_1-q}a_{k_1},\,\mathscr{D}_\nu]\rangle - \sum_{q_1}\lambda_{q_1}[\langle\langle a^\dagger_{k+q+q_1}a_k b_{q_1}a^\dagger_{k_1-q}a_{k_1};\,\mathscr{D}_\nu\rangle\rangle_z +$$

$$+ \langle\langle a^\dagger_{k+q+q_1}a_k b^\dagger_{-q_1}a^\dagger_{k_1-q}a_{k_1};\,\mathscr{D}_\nu\rangle\rangle_z - \langle\langle a^\dagger_{k+q}a_{k-q_1}b_{q_1}a^\dagger_{k_1-q}a_{k_1};\,\mathscr{D}_\nu\rangle\rangle_z -$$

$$- \langle\langle a^\dagger_{k+q}a_{k-q_1}b^\dagger_{-q_1}a^\dagger_{k_1-q}a_{k_1};\,\mathscr{D}_\nu\rangle\rangle_z + \langle\langle a^\dagger_{k+q}a_k a^\dagger_{k_1-q+q_1}a_{k_1}b_{q_1};\,\mathscr{D}_\nu\rangle\rangle_z +$$

$$+ \langle\langle a^\dagger_{k+q}a_k a^\dagger_{k_1-q+q_1}a_{k_1}b^\dagger_{-q_1};\,\mathscr{D}_\nu\rangle\rangle_z - \langle\langle a^\dagger_{k+q}a_k a^\dagger_{k_1-q}a_{k_1-q_1}b_{q_1};\,\mathscr{D}_\nu\rangle\rangle_z -$$

$$- \langle\langle a^\dagger_{k+q}a_k a^\dagger_{k_1-q}a_{k_1-q_1}b^\dagger_{-q_1};\,\mathscr{D}_\nu\rangle\rangle_z] - \delta_{k+q-k_1}(1 - n_k)\left\{\frac{1}{2\pi}\langle[a^\dagger_{k+q}a_{k+q},\,\mathscr{D}_\nu]\rangle +\right.$$

$$+ \sum_{q_1}\lambda_{q_1}[\langle\langle a^\dagger_{k+q}a_{k+q-q_1}b_{q_1};\,\mathscr{D}_\nu\rangle\rangle_z + \langle\langle a^\dagger_{k+q}a_{k+q-q_1}b^\dagger_{-q_1};\,\mathscr{D}_\nu\rangle\rangle_z -$$

$$\left. - \langle\langle a^\dagger_{k+q+q_1}a_{k+q}b_{q_1};\,\mathscr{D}_\nu\rangle\rangle_z - \langle\langle a^\dagger_{k+q+q_1}a_{k+q}b^\dagger_{-q_1};\,\mathscr{D}_\nu\rangle\rangle_z\right\} +$$

$$+ \delta_{k+q-k_1}n_{k+q}\left\{\frac{1}{2\pi}\langle[a^\dagger_k a_k,\,\mathscr{D}_\nu]\rangle + \sum_{q_1}\lambda_{q_1}[\langle\langle a^\dagger_k a_{k-q_1}b_{q_1};\,\mathscr{D}_\nu\rangle\rangle_z +\right.$$

$$\left. + \langle\langle a^\dagger_k a_{k-q_1}b^\dagger_{-q_1};\,\mathscr{D}_\nu\rangle\rangle_z - \langle\langle a^\dagger_{k+q_1}a_k b_{q_1};\,\mathscr{D}_\nu\rangle\rangle_z - \langle\langle a^\dagger_{k+q_1}a_k b^\dagger_{-q_1};\,\mathscr{D}_\nu\rangle\rangle_z\right\}. \quad \text{(A. 2)}$$

The equation of motion for $\langle\langle a^\dagger_{k+q+q_1}b_{q_1}b_q a_k;\,\mathscr{D}_\nu\rangle\rangle_z$ is found to be

$$(z + E_{k+q+q_1} - E_k - \omega_{q_1} - \omega_q)\langle\langle a^\dagger_{k+q+q_1}b_{q_1}b_q a_k;\,\mathscr{D}_\nu\rangle\rangle_z =$$

$$= \frac{1}{2\pi}\langle[a^\dagger_{k+q+q_1}b_{q_1}b_q,\,\mathscr{D}_\nu]\rangle - \sum_{q_2}\lambda_{q_2}[\langle\langle a^\dagger_{k+q+q_1+q_2}a_k b_{q_2}b_{q_1}b_q;\,\mathscr{D}_\nu\rangle\rangle_z +$$

$$+ \langle\langle a^\dagger_{k+q+q_1+q_2}a_k b^\dagger_{-q_2}b_{q_1}b_q;\,\mathscr{D}_\nu\rangle\rangle_z - \langle\langle a^\dagger_{k+q+q_1}a_{k-q_2}b_{q_2}b_{q_1}b_q;\,\mathscr{D}_\nu\rangle\rangle_z -$$

$$- \langle\langle a^\dagger_{k+q+q_1}a_{k-q_2}b^\dagger_{-q_2}b_{q_1}b_q;\,\mathscr{D}_\nu\rangle\rangle_z] + \sum_{k_1}\lambda_{q_1}\langle\langle a^\dagger_{k+q+q_1}a_k a^\dagger_{k_1-q_1}a_{k_1}b_q;\,\mathscr{D}_\nu\rangle\rangle_z +$$

$$+ \sum_{k_1}\lambda_q\,\langle\langle a^\dagger_{k+q+q_1}a_k b_{q_1}a^\dagger_{k_1-q}a_{k_1};\,\mathscr{D}_\nu\rangle\rangle_z. \quad \text{(A. 3)}$$

A similar equation holds for $\langle\langle a^\dagger_{k+q+q_1}b^\dagger_{-q_1}b^\dagger_{-q}a_k;\,\mathscr{D}_\nu\rangle\rangle_z$:

$$(z + E_{k+q+q_1} - E_k + \omega_{q_1} + \omega_q)\,\langle\langle a^\dagger_{k+q+q_1}b^\dagger_{-q_1}b^\dagger_{-q}a_k;\,\mathscr{D}_\nu\rangle\rangle_z =$$

$$= \frac{1}{2\pi}\langle a^\dagger_{k+q+q_1}a_k b^\dagger_{-q_1}b^\dagger_{-q},\,\mathscr{D}_\nu]\rangle - \sum_{q_2}\lambda_{q_2}[\langle\langle a^\dagger_{k+q+q_1+q_2}a_k b^\dagger_{-q_2}b^\dagger_{-q_1}b^\dagger_{-q};\,\mathscr{D}_\nu\rangle\rangle_z +$$

$$+ \langle\langle a^\dagger_{k+q+q_1+q_2}a_k b_{q_2}b^\dagger_{-q_1}b^\dagger_{-q};\,\mathscr{D}_\nu\rangle\rangle_z - \langle\langle a^\dagger_{k+q+q_1}a_{k-q_2}b^\dagger_{-q_2}b^\dagger_{-q_1}b^\dagger_{-q};\,\mathscr{D}_\nu\rangle\rangle_z -$$

$$- \langle\langle a^\dagger_{k+q+q_1}a_{k-q_2}b_{q_2}b^\dagger_{-q_1}b^\dagger_{-q};\,\mathscr{D}_\nu\rangle\rangle_z] - \sum_{k_1}\lambda_{q_1}\langle\langle a^\dagger_{k+q+q_1}a_k a^\dagger_{k_1-q_1}a_{k_1}b^\dagger_{-q};\,\mathscr{D}_\nu\rangle\rangle_z -$$

$$- \sum_{k_1}\lambda_q\,\langle\langle a^\dagger_{k+q+q_1}a_k b^\dagger_{-q_1}a^\dagger_{k_1-q}a_{k_1};\,\mathscr{D}_\nu\rangle\rangle_z. \quad \text{(A. 4)}$$

The quantity $d_3(z)_{k+q,\,k,\,k_1}$ is calculated directly from eq. (3.17). One finds

$$d_3(z)_{k+q,\,k,\,k_1} = \lambda_q^2 \left\{ \frac{1}{z + E_{k+q} - E_k} + \frac{1}{z + E_{k_1-q} - E_{k_1}} \right\} \times$$

$$\times \{u_{k+q,\,k}(\Gamma_{k_1-q,\,k_1,\,q}(z) + \Gamma'_{k_1-q,\,k_1,\,q}(z)) + (\langle a^\dagger_{k_1-q} a_{k_1} b_q \rangle_\lambda +$$

$$+ \langle a^\dagger_{k_1-q} a_{k_1} b^\dagger_{-q} \rangle_\lambda)(G_{k+q}(z) - G_k(z)) + u_{k_1-q\;\,k_1}(\Gamma_{k+q,\,k,\,q}(z) + \Gamma'_{k+q,\,k,\,q}(z)) +$$

$$+ (\langle a^\dagger_{k+q} a_k b_q \rangle_\lambda + \langle a^\dagger_{k+q} a_k b^\dagger_{-q} \rangle_\lambda (G_{k_1-q}(z) - G_{k_1}(z))\} +$$

$$+ \sum_{q_1} \lambda_{q_1}^2 \left\{ \frac{1}{z + E_{k+q} - E_k} + \frac{1}{E_{k+q_1} - E_{k+q+q_1}} \right\} \delta_{k+q+q_1-k_1} \times$$

$$\times \{u_{k+q+q_1,\,k+q}(\Gamma_{k+q_1,\,k,\,q_1}(z) + \Gamma'_{k+q_1,\,k,\,q_1}(z)) +$$

$$+ (\langle a^\dagger_{k+q_1} a_k b_{q_1} \rangle_\lambda + \langle a^\dagger_{k+q_1} a_k b^\dagger_{-q_1} \rangle_\lambda (G_{k+q+q_1}(z) - G_{k+q}(z))\} +$$

$$+ \sum_{q_1} \lambda_{q_1}^2 \left\{ \frac{1}{z + E_{k+q} - E_k} + \frac{1}{E_{k-q_1} + E_{k+q-q_1}} \right\} \delta_{k+q-q_1-k_1} \times$$

$$\times \{u_{k,\,k-q_1}(\Gamma_{k+q,\,k+q-q_1,\,q_1}(z) + \Gamma'_{k+q,\,k+q-q_1,\,q_1}(z)) +$$

$$+ (\langle a^\dagger_{k+q} a_{k+q-q_1} b_{q_1} \rangle_\lambda + \langle a^\dagger_{k+q} a_{k+q-q_1} b^\dagger_{-q_1} \rangle_\lambda)(G_k(z) - G_{k-q_1}(z))\}. \qquad \text{(B. 1)}$$

where

$$u_{k+q,\,k} = n_{k+q} - n_k. \qquad \text{(B. 2)}$$

The evaluation of the correction terms of type $\langle\langle a^\dagger_{k+q+q_1} a_k b_{q_1} b_q ;\, \mathscr{D}_\nu \rangle\rangle_z$ and $\langle\langle a^\dagger_{k+q+q_1} a_k b^\dagger_{-q} b^\dagger_{-q_1} ;\, \mathscr{D}_\nu \rangle\rangle_z$ runs quite analogously. By applying decoupling techniques to the r.h.s. terms of equation (A. 3), one finds

$$\langle\langle a^\dagger_{k+q+q_1} a_k b_{q_1} b_q ;\, \mathscr{D}_\nu \rangle\rangle_z = \lambda_q \lambda_{q_1} \left\{ \frac{1}{z + E_{k+q+q_1} - E_k - \omega_q - \omega_{q_1}} \right\} \times$$

$$\times \{-v_{q_1,\,k+q+q_1} \Gamma_{k+q,\,k,\,q}(z) + \omega_{q_1,\,k} \Gamma_{k+q+q_1,\,k+q_1,\,q}(z) +$$

$$+ w_{q,\,k} \Gamma_{k+q+q_1,\,k+q,\,q_1}(z) - v_{q,\,k+q+q_1} \Gamma_{k+q_1,\,k,\,q_1}(z) -$$

$$-(\langle a^\dagger_{k+q+q_1} a_{k+q_1} b_q \rangle_\lambda + \langle a^\dagger_{k+q+q_1} a_{k+q} b_{q_1} \rangle_\lambda)\, G_k(z) -$$

$$- (\langle a^\dagger_{k+q} a_k b_q \rangle_\lambda + \langle a^\dagger_{k+q_1} a_k b_{q_1} \rangle_\lambda)\, G_{k+q+q_1}(z) +$$

$$+ (\langle a^\dagger_{k+q+q_1} a_{k+q_1} b_q \rangle_\lambda - \langle a^\dagger_{k+q} a_k b_q \rangle_\lambda)\, D_{q_1}(z) +$$

$$+ (\langle a^\dagger_{k+q+q_1} a_{k+q} b_{q_1} \rangle_\lambda - \langle a^\dagger_{k+q_1} a_k b_{q_1} \rangle_\lambda)\, D_q(z)\} +$$

$$+ \lambda_q^2 \delta_{q+q_1} \left\{ \frac{1}{z - 2\omega_q} \right\} \times \sum_{k_1} (\Gamma_{k_1+q,\,k_1,\,q}(z) + \Gamma_{k_1-q,\,k_1,\,-q}(z)) +$$

$$+ (\langle a^\dagger_{k_1+q} a_{k_1} b_q \rangle_\lambda + \langle a^\dagger_{k_1-q} a_{k_1} b_{-q} \rangle_\lambda)\, G_k(z)\}. \qquad \text{(B. 3)}$$

Similarly one obtains from eq. (A .4):

$$\ll a^{\dagger}_{k+q+q_1} a_k b^{\dagger}_{-q_1} b^{\dagger}_{-q}; \mathscr{D}_\nu \gg_z = \lambda_q \lambda_{q_1} \left\{ \frac{1}{z + E_{k+q+q_1} - E_k + \omega_{q_1} + \omega_q} \right\} \times$$

$$\times \{ -w_{q_1, k+q+q_1} \Gamma'_{k+q, k, q}(z) + v_{q_1, k} \Gamma'_{k+q+q_1, k+q_1, q}(z) +$$

$$+ v_{q, k} \Gamma'_{k+q+q_1, k+q, q_1}(z) - w_{q, k+q+q_1} \Gamma'_{k+q_1, k, q_1}(z) +$$

$$+ (\langle a^{\dagger}_{k+q+q_1} a_{k+q_1} b^{\dagger}_{-q} \rangle_\lambda + \langle a^{\dagger}_{k+q+q_1} a_{k+q} b^{\dagger}_{-q_1} \rangle_\lambda) \, G_k(z) +$$

$$+ (\langle a^{\dagger}_{k+q} a_k b^{\dagger}_{-q} \rangle_\lambda + \langle a^{\dagger}_{k+q_1} a_k b^{\dagger}_{-q_1} \rangle_\lambda) \, G_{k+q+q_1}(z) +$$

$$+ (\langle a^{\dagger}_{k+q+q_1} a_{k+q_1} b^{\dagger}_{-q} \rangle_\lambda - \langle a^{\dagger}_{k+q} a_k b^{\dagger}_{-q} \rangle_\lambda) \, D_{q_1}(z) +$$

$$+ (\langle a^{\dagger}_{k+q+q_1} a_{k+q} b^{\dagger}_{-q_1} \rangle_\lambda - \langle a^{\dagger}_{k+q_1} a_k b^{\dagger}_{-q_1} \rangle_\lambda) \, D_q(z)\} +$$

$$+ \lambda_q^2 \delta_{q+q_1} \left\{ \frac{1}{z + 2\omega_q} \right\} \times \sum_{k_1} \{ -n_k (\Gamma'_{k_1+q, k_1, q}(z) + \Gamma'_{k_1-q, k_1, -q})(z) -$$

$$- (\langle a^{\dagger}_{k_1+q} a_{k_1} b^{\dagger}_{-q} \rangle_\lambda + \langle a^{\dagger}_{k_1-q} a_{k_1} b^{\dagger}_{q} \rangle_\lambda) \, G_k(z)\}. \tag{B. 4}$$

APPENDIX C

In this appendix, we shall sketch briefly the derivation of transport equations for a system of electrons, scattered by randomly distributed static impurities, in terms of Green's functions. The Hamiltonian of the electron-impurity system may be written as

$$\mathscr{H}' = \sum_k E_k a^{\dagger}_k a_k + \sum_{k,k'} \lambda V_{kk'} a^{\dagger}_k a_{k'}, \tag{C. 1}$$

where the second term on the r.h.s. describes the electron-impurity scattering. By using the commutation rules

$$[a^{\dagger}_k, \mathscr{H}'] = -E_k a^{\dagger}_k - \sum_{k'} \lambda V_{k'k} a^{\dagger}_{k'} \tag{C. 2}$$

$$[a_k, \mathscr{H}'] = +E_k a_k + \sum_{k'} \lambda V_{kk'} a_{k'} \tag{C. 3}$$

the equation of motion for the Green's function $\ll a^{\dagger}_k a_k; \mathscr{D}_\nu \gg_z$ reads

$$z \ll a^{\dagger}_k a_k; \mathscr{D}_\nu \gg_z = \frac{1}{2\pi} \langle [a^{\dagger}_k a_k, \mathscr{D}_\nu] \rangle + \ll [a^{\dagger}_k a_k, \mathscr{H}']; \mathscr{D}_\nu \gg_z =$$

$$= \frac{1}{2\pi} \langle [a^{\dagger}_k a_k, \mathscr{D}_\nu] \rangle - \sum_{k'} \lambda V_{k'k} \ll a^{\dagger}_{k'} a_k; \mathscr{D}_\nu \gg_z +$$

$$+ \sum_{k'} \lambda V_{kk'} \ll a^{\dagger}_k a_{k'}; \mathscr{D}_\nu \gg_z. \tag{C. 4}$$

This equation is analogous to eq. (3.2) for the electron-phonon system. Instead of higher order Green's functions like $\ll a^{\dagger}_{k+q} a_k b_q; \mathscr{D}_\nu \gg_z$ one obtains in the present case non diagonal Green's functions like $\ll a^{\dagger}_k a_{k'}; \mathscr{D}_\nu \gg_z$. These

latter satisfy in turn equations of motion as

$$(z + E_k - E_{k'}) \langle\langle a_k^\dagger a_{k'}; \mathscr{D}_\nu \rangle\rangle_z = \frac{1}{2\pi} \langle [a_k^\dagger a_{k'}, \mathscr{D}_\nu] \rangle - \\ - \sum_{k''} \lambda V_{k''k} \langle\langle a_{k''}^\dagger a_{k'}; \mathscr{D}_\nu \rangle\rangle + \sum_{k''} \lambda V_{k'k''} \langle\langle a_k^\dagger a_{k''}; \mathscr{D}_\nu \rangle\rangle_z. \qquad \text{(C. 5)}$$

By remarking that $1/2\pi \langle [a_k^\dagger a_{k'}, \mathscr{D}_\nu] \rangle$ corresponds to $C_{kk'}$ and that $\langle\langle a_k^\dagger a_k; \mathscr{D}_\nu \rangle\rangle_z$ and $\langle\langle a_k^\dagger a_{k'}; \mathscr{D}_\nu \rangle\rangle_z$ play respectively the role of f_k and $f_{kk'}$ while $\lambda V_{kk'}$ corresponds to $H'_{k'k}$, one sees that equations (C. 4) and (C. 5) correspond respectively to eqs. (25) and (21) in the paper of Kohn and Luttinger[4]). The first r.h.s. term of eq. (C. 5) is the analogon of the first r.h.s. terms $\langle [a_{k+q}^\dagger a_k b_q, \mathscr{D}_\nu] \rangle$ and $\langle [a_{k+q}^\dagger a_k b_{-q}^\dagger, \mathscr{D}_\nu] \rangle$ of eqs. (3.4) and (3.5). By going back into (A.4) one sees that the first r.h.s. term of eq. (A.5) yields a contribution

$$\sum_{k'} \left[\lambda V_{kk'} \frac{\langle [a_k^\dagger a_{k'}, \mathscr{D}_\nu] \rangle}{z + E_k - E_{k'}} \right], \qquad \text{(C. 6)}$$

being equivalent to the term

$$\sum_{k'} \left[\frac{C_{kk'} H'_{k'k}}{d_{kk'}} \right]$$

in eq. (81) of Kohn and Luttinger[4]) and which is comparable to our interference terms $F^e_{2;k}(z)$ eq. (4.26).

Received 23-6-64

REFERENCES

1) Michel, K. H. and Van Leeuwen, J. M. J., Physica **30** (1964) 410.
2) Zubarev, D. N., Sov. Phys. Uspekhi **3** (1960) 320.
3) Bogoljubov, N. N., Studies of Statistical Mechanics; edited by J. de Boer en G. E. Uhlenbeck (North-Holland, Amsterdam, 1962).
4) Kohn, W. and Luttinger, J. M., Phys. Rev. 108 (1957) 590.
5) Verboven, E., Physica **26** (1960) 1091.
6) Bloch, C. and De Dominicis, C., Nuclear Phys. **7** (1958) 459.
7) Nishikawa, K. and Barrie, R., Canad. Journ. of Phys. **41** (1963) 1135.
8) Bogoljubov, N. N. and Tyablikov, S. V., Soviet Phys. Doklady **4** (1959) 589.
9) Berger, P., Van Leeuwen, J. M. J. and Verboven, E., Physica **29** (1963) 1409.
10) Kadanoff, L. and Baym, G., "Quantum Statis. Mechanics", (Benjamin Inc. 1962).
11) Michel, K. H. and Verboven, E., Physics Letters **8** (1964) 176.
12) Cohen, E. G. D., in Fundamental "Problems in statist. Mechanics", (North-Holland 1962).
13) Van Leeuwen, J. M. J., to appear in Physica.
14) Ron, A., Journ. math. Phys. **4** (1963) 1182.
15) Wyld, H. W. and Fried, B. D., Annals of Physics **23** (1963) 374.
16) Davis, H. I. and Résibois, P., J. chem. Phys. **40** (1964) 3276.

MOTIVERING EN SAMENVATTING

De beschrijving van transport-verschijnselen van electronen en phononen in metalen en halfgeleiders werd in het algemeen gebaseerd op de theorie van de Boltzmann vergelijking. Hierbij neemt men aan, dat de verdelingsfuncties $f^e(k)$ van de electronen en $f^p(q)$ van de phononen voldoen aan de volgende vergelijkingen:

$$\frac{\partial f^e}{\partial t}(\boldsymbol{k}, t) = -\frac{e\boldsymbol{E}}{m}\frac{\partial f^e}{\partial \boldsymbol{k}}(\boldsymbol{k}, t) + \left(\frac{\partial f^e}{\partial t}(\boldsymbol{k}, t)\right)_{\text{botsing}} \tag{1}$$

$$\frac{\partial f^p}{\partial t}(\boldsymbol{q}, t) = \left(\frac{\partial f^p}{\partial t}(\boldsymbol{q}, t)\right)_{\text{botsing}} \tag{2}$$

De eerste term van het rechter lid van (1) geeft de verandering van de verdeling van de electronen aan, veroorzaakt door het uitwendig electrische veld $\boldsymbol{E}$ (e is de lading van het electron, m zijn massa en $\boldsymbol{k}$ zijn impuls). De tweede term beschrijft de verandering van f^e, veroorzaakt door de botsing van de electronen met de phononen van het rooster.

Bij vergelijking (2) voor de verdelingsfunctie $f^p(\boldsymbol{q})$ van de phononen (waarin $\boldsymbol{q}$ de phonon-golfvector is) is er geen directe werking van het uitwendig veld en worden de phononen slechts uit hun evenwicht gebracht door hun botsingen met de electronen. In het stationaire geval verdwijnt de linker term van (1) en de rechter termen laten zien, dat het effect van het uitwendig veld door de botsingen tussen electronen en phononen wordt tegengewerkt. Bij het oplossen van vergelijking (1) neemt men voor $f^e(\boldsymbol{k})$ in de eerste term van het rechter lid van (1) de ongestoorde Fermi-Dirac verdeling $f_0^e(\boldsymbol{k})$, terwijl de botsingsterm gewoonlijk door tweede orde storingstheorie berekend wordt. De botsingsterm in vergelijking (2) voor phononen wordt op dezelfde wijze behandeld. Als resultaat krijgt men dan de welbekende Boltzmann vergelijkingen voor electronen en phononen[1])*), die van de tweede orde zijn in de electron-phonon koppeling λ_q. Tegen de

*) Zie referenties bij hoofdstuk I

zojuist beschreven methode zijn verschillende bezwaren aan te voeren[1)2)].

Ten eerste: de methode waarmee men de botsingstermen in de vergelijkingen (1) en (2) berekent. De daarvoor benodigde overgangswaarschijnlijkheden zijn afgeleid door middel van tijdsafhankelijke verstrooiingstheorie van laagste orde, een methode, die alleen juist is voor voldoende korte tijdsintervallen Δt. Het gebruik van tijdsonafhankelijke overgangswaarschijnlijkheden op elk tijdstip t in de botsingsterm wordt dan plausibel gemaakt door argumenten, die "random phase" benaderingen en veronderstellingen over de botsingstijd bevatten. In het bijzonder gaat men er hierbij van uit, dat de botsingstijd korter is dan de tijd tussen twee opeenvolgende botsingen. Door de laatste benadering wordt men er toe geleid een andere moeilijkheid van de Boltzmannvergelijking te beschouwen. In vergelijking (1) neemt men aan dat de botsingsterm niet beinvloed wordt door het uitwendig veld, met andere woorden, het uitwendig veld wordt verondersteld alleen op deeltjes te werken die vrij zijn tussen de botsingen: de werking van het veld gedurende de botsingen wordt hierdoor verwaarloosd.

Ten einde de zoëven genoemde moeilijkheden te vermijden en een meer exacte theorie van transportverschijnselen te geven, dient men uit te gaan van andere uitdrukkingen dan verg. (1) en (2).

Een algemene formule die de responsie van een systeem op een uitwendige storing beschrijft, is door Kubo[3)] gegeven. Zijn behandeling is gebaseerd op de beschrijving van de verandering van de dichtheidsmatrix van het systeem als gevolg van het uitwendig veld.

Als de uitwendige storing voldoende zwak is, is het gerechtvaardigd om slechts de lineaire responsie functie te beschouwen, die kan worden uitgedrukt in een twee-tijds correlatiefunctie. In het bijzonder kan de electrische weerstand worden beschreven als een correlatiefunctie van twee stromen. Deze vorm van de Kubo formule werd door Chester en Thellung[4)] en Verboven[5)] gebruikt bij een onderzoek van transportverschijnselen voor electronen in wisselwerking met onzuiverheden. Kohn en Luttinger[6)] bestudeerden dit probleem met een andere methode, die gebaseerd is op de dichtheidsmatrix van één electron. Al deze onderzoekingen werden vereenvoudigd door het feit dat het gerechtvaardigd was om slechts één electron in wisselwerking met een systeem van willekeurig verdeelde statische onzuiverheden te beschouwen. In het geval van electron-phonon verstrooiing is de situatie ingewikkelder. Men heeft te maken met een echt veeldeeltjesprobleem en de technieken, die gebruikt zijn in de bovengenoemde artikelen zijn minder toepasselijk.

In de laatste jaren zijn veldtheoretische methodes met groot succes in de vaste stoffysika en in de statistische mechanika toegepast. De Green's functie techniek bleek daarbij de meest effectieve methode te zijn en is geschikt voor evenwichts- zowel als voor transportproblemen in de statistische fysika[7)].

In hoofdstuk twee van dit proefschrift beschouwen we niet de Kubo formule in zijn gewone vorm maar gaan we uit van een uitdrukking die al eerder in de afleiding van de Kubo formule voorkomt. Dit laat ons toe de electrische geleiding onmiddellijk in de Fourier getransformeerde van de geretardeerde Green's functie uit te drukken. Deze Green's functie is te interpreteren als de verandering van de electrondistributie veroorzaakt door het uitwendig veld. Ze speelt de rol van de lineaire afwijking (in $\boldsymbol{E}$) van de functie $f^e(\boldsymbol{k})$ in de gewone Boltzmann vergelijking ten opzichte van zijn evenwichtswaarde $f_0^e(\boldsymbol{k})$. Uitgaande van een "elementaire" Green's functie $G_{\boldsymbol{k}}$ kunnen we, door de bewegingsvergelijkingsmethode voor Green's functies toe te passen, een hiërarchie voor de Green's functies afleiden. Deze hiërarchie bevat gemengde electron-phonon Green's functies van hogere orde. Zoals bekend uit de algemene theorie, moeten we de hiërarchie door bepaalde benaderingsmethodes afbreken. In ons probleem doen we dit met behulp van de zogenaamde ontkoppelingstechniek, een methode die het eerst werd toegepast door Bogoljubov en Tyablikov[7][8]). Op deze manier verkrijgen wij een lineaire integraal-vergelijking voor $G_{\boldsymbol{k}}$ en voor $D_{\boldsymbol{q}}$, waar laatstgenoemde Green's functie de lineaire afwijking is van de phonon distributie. Deze termen, die op een natuurlijke wijze in onze berekeningen verschijnen, staan bekend als "phonon drag". In het geval van een statisch electrisch veld is ons systeem van twee gekoppelde integraal-vergelijkingen voor $G_{\boldsymbol{k}}$ en $D_{\boldsymbol{q}}$ equivalent met de gelineairiseerde versie van de Bloch-Boltzmann vergelijkingen voor electronen en phononen. De inhomogene term in de vergelijking voor $G_{\boldsymbol{k}}$ is identiek met de gewone stromingsterm van de Boltzmann vergelijking terwijl het homogene gedeelte correspondeert met de botsingsterm die van tweede orde in de electron-phonon koppeling is. Dit laat duidelijk zien, dat de scheiding tussen stromings- en botsingstermen, zoals gemaakt in vergelijking (1) in laagste orde van de electron-phonon interactie, gerechtvaardigd is. Het laatste deel van hoofdstuk II is gewijd aan de discussie over de behoudswetten van energie, totaal impuls en aantal electronen. De behoudswetten worden zowel gegeven voor de exacte kinetische vergelijkingen (van elke orde in de electron-phonon interactie) als voor de kinetische vergelijkingen, verkregen na ontkoppeling. Bij afwezigheid van „Umklapprozesse" is de totale impuls een behouden grootheid en de electrische geleiding wordt oneindig. Dit is een bekend gevolg van de phonon drag. Tenslotte worden de kinetische vergelijkingen opgeschreven, door „Umklapprozesse" in rekening te brengen. Daardoor worden de behoudswetten gewijzigd en de electrische geleiding blijft eindig.

Het volgende hoofdstuk is een uitbreiding tot hogere orde in de electron-phonon interactie. Ten eerste wordt de Green's functie-hierarchie tot de vierde orde afgeleid. Door ontkoppeling in dit stadium verkrijgt men opnieuw de resultaten van orde $\lambda_{\boldsymbol{q}}^2$ berekend in hoofdstuk II en additionele

termen, die van hogere orde zijn in de electron-phonon interactie. Men krijgt twee hoofd-klassen van correcties.

Eerst zijn er de correcties aan de botsingsterm (orde λ_q^4), die gegeven worden door het homogene deel van de integraal vergelijking. Hier kan men opnieuw onderscheid maken in twee groepen. Het eerste deel van de termen brengt de renormalisatie van de electron- en phonon-energie en correcties aan de overgangswaarschijnlijkheden in rekening. Het overblijvende gedeelte van de correcties aan de botsingsterm bevat electron-phonon dichtheidsmatrices als gevolg van correlatie effecten, die kenmerkend zijn voor het veeldeeltjeskarakter van het systeem.

De tweede groep van correcties is van geheel andere aard en verdient speciale aandacht. In de vergelijking voor de electron Green's functie G_k verkrijgt men behalve de bekende stromingsterm een hele klasse van termen, die veroorzaakt zijn door de interferentie tussen stroming en botsing. Deze termen behoren tot het niet homogene deel van de integraal vergelijking en zijn evenredig met de uitwendige storing. Anderszijds zijn ze ook evenredig met de electron-phonon interactie (in ons geval van orde λ_q^2) en bevatten andere factoren, die veroorzaakt zijn door de botsing. Deze interferentietermen worden veroorzaakt door de werking van het electrische veld gedurende botsingen. De deeltjes worden hier niet langer beschouwd als zich vrij bewegend tussen ogenblikkelijke botsingen. Een zelfde soort correcties is ook aanwezig in de kinetische vergelijking voor phononen, die in het algemeen (in de laagste orde beschouwd) geen stromingsterm bevat. Onze resultaten tonen aan, dat het schema zoals gegeven door vergelijking (1) en (2) alleen gerechtvaardigd is in de laagste orde in de electron-phonon interactie en dat het niet geldig is in een meer correcte formulering van transportverschijnselen.

Hoofdstuk II en III zijn als afzonderlijke artikelen in Physica opgenomen; hoofdstuk II in Physica 30, blz. 410 (1964), hoofdstuk III in druk.

STELLINGEN

I

Indien men de botsingsdoorsneden van zware molekulen aan zware atomen meet voor twee ongelijke magnetische rotatie kwantumgetallen, dan levert het verschil hiervan goed te analyseren informatie over de assymetrie van het attraktieve gedeelte van de intermolekulaire potentiaal

H G Bennewitz, K H Kramer, W Paul en J P. Toennies, Z f Phys **177** (1964) 84–110

II

Recente metingen van Pavlov, Damiljan en Kozolkov van het vervalschema van In 116 zijn niet exakt

Pavlov et al Bull Acad Sc USSR vol **27**, no 7 (1963) 884

P Fettweis en J Vervier, Physics Letters **3** (1962) 36

III

Wegens het toenemend belang van wetenschappelijke russische publikaties is het wenselijk, dat een cursus in de russische taal deel uitmaakt van de postdoktorale opleiding

IV

Het verdient aanbeveling, de eigenschappen van polaronen (speciaal wat betreft de effektieve massa en de energie als funktie van de snelheid) met behulp van de inelastische verstrooiing van neutronen aan polaire kristallen te onderzoeken

J J J Kokkedee, Physica **28** (1962) 893

V

Bij het berekenen van hoger dan eerste orde korrekties op de massa's van elementaire deeltjes, behorende tot eenzelfde SU_3 representatie, is het nodig daarbij rekening te houden met een mogelijke menging van verschillende representaties

S Okubo, Physics Letters **4** (1963) 14

VI

De afleiding van formule (5.29) in "Relativistic kinematics" van R. Hagedorn voor de maximale hoek van een impulsspektrum na een Lorentztransformatie van het zwaartepunt-systeem naar het laboratorium-systeem is niet korrekt.

R. Hagedorn, Relativistic Kinematics p 53, (5 29) Benjamin (1963)

VII

De veel voorkomende uitdrukking, die de temperatuurafhankelijkheid van koolweerstanden beschrijft, is op dimensionale gronden onjuist.

von Angerer-Ebert, Technische Kunstgriffe bei physikalischen Untersuchungen, Vieweg, Braunschweig (1959)

VIII

Voor lage frequenties van het uitwendig veld kan men vergelijking (4.8) in hoofdstuk II van dit proefschrift oplossen. Verwaarloost men de fonon drag termen dan krijgt men voor de elektrische geleiding een uitdrukking, die dezelfde vorm heeft als de Drude formule voor wisselstroom.

P Drude, Annalen der Physik **14** (1904) 936.

22 januari 1965 K. H. Michel